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## **Mini-Workshop: Lorentz Gas Dynamics: particle systems and scaling limits**

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**ABSTRACT.** This workshop had the aim to bring together leading experts from different fields, i.e. interacting particle systems, dynamical systems and kinetic theory, to consider questions related to the dynamics of the Lorentz gas and to promote the exchange of information concerning the techniques that have been developed in different contexts and communities.

*Mathematics Subject Classification (2010):* 82B40, 82C05, 76P05, 35Q20, 35Q84, 82D05, 70F45, 82C22, 37A60, 35B27, 82C70, 60J60, 60J65, 35Q70 .

### **Introduction by the Organizers**

The mini-workshop Lorentz Gas Dynamics: particle systems and scaling limits, organised by Alessia Nota (Bonn), Chiara Saffirio (Zürich) and Juan Velázquez (Bonn) gathered together 18 participants, including the organisers, with broad geographic and thematic representation. Indeed, being the Lorentz gas a prototype model in the derivation of effective equations from Hamiltonian mechanics, it has been approached by several different mathematical communities using different mathematical tools from statistical mechanics to probability, from analysis to number theory. The main goal successfully achieved in the workshop was to strengthen the bridge among the communities of interacting particle systems, dynamical systems, kinetic theory and quantum mechanics.

The format of the workshop consisted of two to four one-hour lecture per day, thus leaving several free slots for spontaneous discussions. Such free time was very important for people from different communities to get to know each other, deepening the arguments of the lectures and developing new scientific interactions.

Young researchers especially benefit from it. Incidentally we underline that different scientific ages were represented, with a significant number of women and young participants.

The workshop developed around the following main themes: validity of the linear Boltzmann equation under different scatterers distributions; fluctuations; nonlinear models; quantum many-body systems.

Concerning the linear models, a very interesting and highly animated talk has been given by Bernt Wennberg, who reviewed the known results and open problems on the Lorentz model with scatterer distributions different from Poisson and made some conjectures supported by numerical simulations. Closely, Raphael Winter provided a rigorous derivation of a linear Boltzmann equation with annihilation, in the Boltzmann-Grad limit, from an ideal Rayleigh Gas with annihilation, while Christopher Lutsko proved an invariance principle and a central limit theorem for the Lorentz Gas in dimension 3 considering simultaneously the Boltzmann-Grad kinetic limit and diffusive scaling.

Fluctuations around the effective dynamics were analysed in the talks by Giada Basile and Sergio Simonella. Giada Basile presented a gradient flow approach for the linear Boltzmann equation arising from a Lorentz model and the large deviation asymptotics of a Kac random walk with bounded velocities, whereas Sergio Simonella presented a work in progress concerning dynamical fluctuations around the nonlinear Boltzmann equation, showing that a central limit theorem holds in the low-density limit of a hard-sphere system.

A majority of the contributions were devoted to nonlinear models. They included: some numerical simulations and analytical study of the limits at different scales of the Uchiyama model presented by Nathalie Ayi; a microscopic approach to classical quadratic models of cross diffusion appearing in population dynamics, showing that the solutions of these models can be obtained as limits of solutions of microscopic models in some suitable limit presented by Laurent Desvillettes; entropy inequalities for the Kac model providing new estimates on the rate of convergence to equilibrium presented by Maria C. Carvalho. On the same topic, Eric Carlen and Mario Pulvirenti focused on thermodynamical properties of non-equilibrium steady states for open systems in kinetic theory, respectively for the BGK model and for the nonlinear stationary Boltzmann equation. These talks were followed by several discussions that will certainly lead to future progresses.

The theme of many-body quantum systems has been addressed by: Giulia Basti, who presented a quantum Lorentz gas with Gross-Pitaevskii potential which exhibits a universal behaviour for large  $N$ ; François Golse, who introduced the new notion of quantum empirical measures with a clear correspondence between classical and quantum objects, thus making easier for the participants from outside the quantum community to understand and appreciate the powerfulness of these new mathematical objects; Jory Griffin, who gave a talk on quantum transport in a low-density periodic potential showing that the time evolution of a quantum wave packet in a periodic potential converges in a combined high-frequency Boltzmann-Grad limit, up to second order in the coupling constant, to terms

that are compatible with the linear Boltzmann equation; Nikolai Leopold, who focused on a quantum system of non-relativistic fermions coupled to a zero mass quantized scalar field, proving that the time evolution in a coupled mean-field and semiclassical limit of many fermions can be approximated by the fermionic Schrödinger-Klein-Gordon equations.

Finally, the talk by Massimiliano Gubinelli – followed by stimulating discussions – reviewed the theory of rough paths, which could be a new, powerful technique to approach kinetic models. In particular, he presented some perspectives concerning the derivation of the linear kinetic equations from the random Schrödinger equation with a homogeneous random potential (Quantum Lorentz Gas).

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## Abstracts

### Numerical Study of the Uchiyama particle model

NATHALIE AYI

The physical context that we are interested in is the one of the kinetic theory of gases. There exists several levels of description for this one: the microscopic, the mesoscopic and the macroscopic scales. The famous sixth problem of Hilbert is about linking these different scales. More specifically, it suggests to use the Boltzmann equation as an intermediate step in the transition between atomistic and continuous models for gas dynamics. The historical result addressing this question is due to Lanford [10] who established the convergence in the low density limit to the Boltzmann equation, starting from the particle system called hard spheres (only for short times). Until the end of the 90's, the proof of Lanford has been completed by many authors. More recently, the proof has been improved by means of quantitative estimates by Gallagher, Saint-Raymond, Texier [8], Pulvirenti, Saffirio, Simonella [12]. Recent improvements regarding the linear setting have been also made (Bodineau, Gallagher, Saint-Raymond[4], Ayi [2], ...).

We take an interest in a variant of this setting: discrete velocity models (DVM). It consists in models involving particles which can take only a finite number of velocities. The model we are interested in is the Broadwell one [5]: we define the set  $S$  as follows

$$(1) \quad S := \{v_1, v_2, v_3, v_4\},$$

with  $v_1 := (1, 0)$ ,  $v_2 := (-1, 0)$ ,  $v_3 := (0, 1)$ ,  $v_4 := (0, -1)$  and we study the equation

$$(2) \quad \partial_t f(t, x, v) + v \cdot \partial_x f(t, x, v) = a[f(t, x, iv)f(t, x, -iv) - f(t, x, v)f(t, x, -v)]$$

with  $t \in \mathbf{R}^+$ ,  $x \in \mathbf{R}^2$ ,  $v \in S$ ,  $a$  a nonnegative constant and where  $i$  denotes the  $\pi/2$  rotation operator. The two natural microscopic models which would be the equivalent of the hard spheres for discrete velocities are the HPP model [9] introduced by de Hardy, Pomeau et de Pazzis and the Uchiyama model [13]. The first one is a lattice model while the second one is continuous.

The HPP model describes the evolution of particles on a lattice in dimension two with particles which have their velocities living in  $S$ . The description of the dynamics is the following: during one unit of time, each particle jumps in the direction of its velocity. At each site where the number of particles is two and where two particles have opposite velocities, there is a collision, and each velocity turns with an angle of  $\pi/2$ . For all the other sites, nothing changes.

The Uchiyama model describes the evolution of “hard” squares in  $\mathbf{R}^2$  whose diagonals are of length  $\varepsilon$  and parallel (or orthogonal) to the coordinate axes. Particles move freely with velocities belonging to  $S$  until they undergo a collision. We distinguish two types of collision: the “head-on” collisions and the “side-to-side” ones. The collision rules are the following: in case of a “side-to-side” collision,

the particles involved exchange their velocities while in case of a “head-on”, the velocities undergo a rotation of angle  $\pm\pi/2$ .

Surprisingly, Uchiyama proved in [13] that, except for very particular situations, in the low density limit, starting from his model, we do not obtain the Broadwell equation. The same applies to the HPP model. The question of the limit model associated with the Uchiyama one is then open. Indeed, one of the inherent difficulties of those DVM models is the appearance of a phenomenon of recollisions between the particles which cannot be controlled. Therefore, if a kinetic equation exists, it should contain a memory term associated with this phenomenon. Nevertheless, up to now, it is a very difficult problem and there is not much more which is known. This is why we have decided, in a first place, to adopt a numerical approach.

We carry out the molecular dynamics simulation for the Uchiyama’s particle system using an Event-Driven algorithm. The Event-Driven method is concerned with the times at which events, in this case collisions, take place. The algorithm is the following: you establish a list of the collisions to come if the particles moved only in straight lines. This list is ordered according to the time at which the collisions will take place, the first element being the closest collision in time. The particles are then displaced until this time and the collision is carried out. The list of future collisions is then updated. Indeed, some of them may be invalidated by the collision that has just taken place since the velocities and therefore the direction of the two particles involved have changed, new ones may also become possible for the same reasons. Then, again, we move to the nearest collision in time and so on ...

First, we take an interest in the low density limit, the one for which we fail to obtain the Broadwell equation. In that case, in the spirit of the paper of Aoki et al [1] in the hard spheres case, we study the backward cluster. A backward cluster is defined as the group of particles involved directly or indirectly in the backwards-in-time dynamics of a given tagged sphere. We denote  $J_i = \{i_1, i_2, \dots, i_n\}$  with  $i_r \neq i_s$  for  $i \neq s$  the backward cluster of the particle  $i$ ,  $K_i = |J_i|$  the cardinality of  $J_i$ . We are interested in  $\langle K \rangle_t$  the average with respect to the initial position of the cardinality of the backward cluster of a tagged particle at time  $t$ . We focus on the quantity

$$r = \lim_{t \rightarrow \infty} \frac{1}{t} \log(\langle K \rangle_t + 1).$$

Our preliminary result shows that, as in[1], we should obtain an exponential estimate of the growth in time of  $\langle K \rangle_t$  for the Uchiyama model, with a different  $r$  than for the hard spheres.

We introduce the notion of internal and external recollisions: internal recollisions (recollision in the pseudo-trajectory sense in the backward trajectory of a particle), and external recollisions (when the two backward clusters of two particles have a non-empty intersection). Thus, for  $N$  particles and  $M$  trajectories, we

are interested in the two quantities:

$$P^{i.r.} = \frac{1}{N} \frac{1}{M} \sum_{m=1}^M \sum_{i=1}^N \mathbf{1}_{\{\text{particle } i \text{ presents a recollision on the } m\text{-th trajectory}\}}$$

and

$$P^{e.r.} = \frac{1}{M} \frac{1}{\frac{N(N-1)}{2}} \sum_{m=1}^M \sum_{1 \leq i < j \leq N} \mathbf{1}_{\{\text{particle } i \text{ and particle } j \text{ undergo an external recollision}\}}.$$

We think that, most of the time, there is propagation of chaos, except exactly where we would need to have it to obtain the Broadwell equation. Therefore, we expect  $P^{i.r.}$  not to be small and, on the contrary,  $P^{e.r.}$  to be small for the Uchiyama model, while it is clear that it is small in both cases for the hard spheres model. The results numerically obtained goes exactly in that direction.

**Uchiyama**

**Hard Spheres**

$N$	$t$	$\langle K \rangle_t$	$P^{i.r.}$	$P^{e.r.}$
3000	1	7	0.16	0.02
4000	1	7.8	0.15	0.02
5000	1	7.8	0.15	0.01
8000	1	7	0.15	0.008
10000	1	7.8	0.15	0.006
12000	1	7.6	0.14	0.005

$N$	$t$	$\langle K \rangle_t$	$P^{i.r.}$	$P^{e.r.}$
3000	1	7.3	0.02	0.02
4000	1	7	0.02	0.01
5000	1	7	0.02	0.01
8000	1	7	0.01	0.007
10000	1	7	0.01	0.006
12000	1	7	0.01	0.005

$N$	$t$	$\langle K \rangle_t$	$P^{i.r.}$	$P^{e.r.}$
3000	1.9	14.8	0.30	0.07

$N$	$t$	$\langle K \rangle_t$	$P^{i.r.}$	$P^{e.r.}$
3000	1.9	13.7	0.05	0.06

$N$	$t$	$\langle K \rangle_t$	$P^{i.r.}$	$P^{e.r.}$
3000	2.8	21.6	0.43	0.14

Finally, in a last part, we observe a regime which seems close enough from the diffusive limit. We recall that for the hard-spheres, the limit process is a Brownian motion. Of course, regarding our previous remarks, we have no hope to obtain such a process for our diffusive limit. We numerically test a wider class: fractional Brownian motion. Our preliminary results indicate that the limit process does not belong to that class either.

From a theoretical point of view, there are many paths that we plan to explore.

- We could as in [6] work in an extended phase space. The good new set of parameters would be given by the one which allows to make appear the pathological structures (two particles moving one ahead of the other one in the same direction).

- We could put an additional term catching all the pathological situations (like the “flowers” appearing in the case of the Two-Dimensional Magnetotransport equation, see [3]).
- We could also rescale in time and take an interest in the super diffusion limit as in [11] to obtain the usual limit process.
- We could study a version with randomness of the Uchiyama model for which one we could hope to obtain the Broadwell equation (as it is the case for the HPP model, see [7]).

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**Large deviations for some linear kinetic equations**

GIADA BASILE

Linear Boltzmann equations, such as the Boltzmann-Grad limit for the Lorentz gas, have the following general form

$$(\partial_t + b(v) \cdot \nabla_x) f(t, x, v) = \int_{\mathcal{V}} \pi(dv') \sigma(v, v') [f(t, x, v') - f(t, x, v)],$$

where  $\pi(dv)$  is a probability measure on the velocity space  $\mathcal{V}$ ,  $b$  is the drift,  $\sigma(v, v') = \sigma(v', v) \geq 0$  is the scattering kernel and  $f$  is the density of the one-particle distribution with respect to  $dx \pi(dv)$ . The condition on  $\sigma$  follows from a reversibility assumption. The velocity space  $\mathcal{V}$  can be either  $\mathbb{R}^d$ ,  $\mathbb{T}^d$ ,  $\mathbb{S}^{d-1}$ , or a discrete state space. We assume that the position space is the  $d$  dimensional torus. From a probabilistic point of view, the equation is the Fokker-Planck equation of the process  $(V(t), X(t))_{t \geq 0}$  where  $V(\cdot)$  is an autonomous jump process, taking value in  $\mathcal{V}$ , with jump rate  $\pi(dv') \sigma(v, v')$  and  $X(\cdot)$  is an additive functional of  $V$ , namely  $X(t) = \int_0^t b(V_s) ds$ .

Given  $N$  independent copies of the process  $(V(t), X(t))_{t \geq 0}$ , one can construct the empirical measure  $\alpha_t^N(dx, dv) = \frac{1}{N} \sum_{i=1}^N \delta_{X^i(t)}(dx) \delta_{V^i(t)}(dv)$ . The associated linear Boltzmann equation (LBE) is the law of large numbers of the empirical measure in the limit  $N \rightarrow \infty$ .

We would like to investigate large deviations, i.e. the asymptotic probability that the empirical measure differs from the typical one  $f_t dx d\pi$ , with  $f_t$  solution to the LBE. To this aim it is convenient to consider the current as a dynamical variable. Set  $\eta^f = \sigma(v, v') [f(t, x, v) - f(t, x, v')]$ , then LBE can be rewritten as

$$\begin{cases} (\partial_t + b(v) \cdot \nabla_x) f(t, x, v) + \int \pi(dv') \eta(t, x, v, v') = 0, \\ \eta = \eta^f \end{cases}$$

where the first equation plays the role of a continuity equation. Together with the empirical measure consider the empirical current  $Q^N(dt, dx, dv, dw)$  as

$$Q^N(F) = \frac{1}{N} \sum_{i=1}^N \sum_k F(\tau_k^i, X^i(\tau_k^i), V^i(\tau_k^{i-}), V^i(\tau_k^i)),$$

for every  $F \in C([0, T] \times \mathbb{T}^d \times V \times V)$  anti-symmetric in the exchange of the velocities. The following continuity equation holds

$$\alpha_t^N(\phi) - \alpha_0^N(\phi) = \frac{1}{N} \sum_{i=1}^N \sum_{k \geq 0} [\phi(X^i(\tau_k^i), V^i(\tau_k^i)) - \phi(X^i(\tau_k^i), V^i(\tau_k^{i-}))],$$

for any  $\phi: \mathbb{T}^d \times V \rightarrow \mathbb{R}$  continuous and bounded. Assume at time zero  $\{V^i(0), X^i(0)\}$  iid with law  $\nu$ . For every couple  $(\mu, \Theta)$  (measure and current) satisfying the continuity equation, one expects the following asymptotics

$$\mathbb{P}_\nu [(\alpha^N, Q^N) \sim (\mu, \Theta)] \sim e^{-N I(\mu, \Theta)},$$

with an action functional  $I(\mu, \Theta) = H(\mu_0|\nu) + J(\mu, \Theta)$ . Here the first term is the relative entropy with respect to the initial distribution and

$$J(\mu, \Theta) = \int_0^T dt \int dx \iint_{\mathcal{V} \times \mathcal{V}} \pi(dv)\pi(dw)\Phi_\sigma(g(t, x, v), g(t, x, w), \zeta(t, v, w)),$$

where  $d\mu_t = g(t)d\pi$ ,  $d\Theta = \zeta(t)dt d\pi \otimes d\pi$  and  $\Phi$  is a convex, positive function which is equal to zero iff the couple  $g, \eta$  satisfies the LBE. The statement can be easily proved at least in the homogeneous case, i.e. the drift  $b = 0$  and  $f$  depending only on time and velocity, under suitable assumption on the jump rate.

In a work in progress together with D. Benedetto, L. Bertini and C. Orrieri we investigate the large deviation asymptotics for a Kac-like walk, which is described at the kinetic level by a non linear homogeneous Boltzmann equation. At the microscopic level, at random times two particles with velocities  $v$  and  $v_*$  “collide” and change their velocities in such a way the total momentum is preserved, i.e., denoting by  $v', v'_*$  their velocities after collision,  $v + v_* = v' + v'_*$ .

We expect that the action function is similar to the previous one, but now with the function  $\Phi$  computed on the product of the densities, namely  $\Phi_\sigma(gg_*, g'g'_*, \zeta)$ , where, using the usual kinetic notations,  $g_* = g(t, v_*)$ ,  $g'_* = g(t, v'_*)$ . The solution to the homogeneous Boltzmann equation is then the zero level set of the rate function.

## Universal low-energy behavior in a quantum Lorentz gas with Gross-Pitaevskii potentials

GIULIA BASTI

(joint work with S. Cenatiempo, A. Teta)

Consider a quantum particle moving in three dimensions through a large number of randomly distributed obstacles whose dimension is much smaller than the average distance among them. If the energy of the particle is sufficiently small we can assume its wavelength to be much larger than the two above mentioned length scales. Under these assumptions, which describes situations emerging in physical contexts such as scattering of slow neutrons from condensed matter, one reasonably expects that the details of the interaction become irrelevant and the behavior of the system can be characterized using only few physical parameters exhibiting what is called a *universal behavior*.

In this talk I report a work in collaboration with S. Cenatiempo and A. Teta [1] where we give a rigorous proof of this expectation. In our description we model the obstacles rescaling a potential  $V \in L^1(\mathbb{R}^3, (1 + |x|^4)dx) \cap L^3(\mathbb{R}^3)$  defining

$$(1) \quad V_i^N(x) = N^2 V(N(x - y_i))$$

where the positions  $\{y_i\}_{i=1, \dots, N}$  of the  $N$  obstacles are assumed to be independent and identically distributed random variables with common density  $W$ . Obviously,  $W \geq 0$  and  $\int W(x)dx = 1$ . In addition, we ask  $W \in L^1(\mathbb{R}^3) \cap L^p(\mathbb{R}^3)$  for some  $p > 3$ .

The scaling defined in (1) is known as Gross-Pitaevskii scaling and describes rare (the range of the interaction scales as  $N^{-1}$ ) but strong (due to the factor  $N^2$  in front of the interaction) interactions. It's worth noticing, in particular, that the range of the interaction is much smaller than the average distance among the particles (which is of order  $N^{-1/3}$ ) and hence it is suitable to describe the regime of our interest. The evolution of the particle is then given by the Hamiltonian operator in  $L^2(\mathbb{R}^3)$

$$(2) \quad H_N = -\Delta + \sum_{i=1}^N V_i^N(x)$$

where we set  $\hbar = 1$  and we are assuming the particle to have mass  $1/2$ .

Rewriting the interaction term as  $\frac{1}{N} \sum_{i=1}^N w_i^N(x)$  we have that  $w_i^N(x) = N^3 V(N(x - y_i))$  converges toward a delta distribution in the limit  $N \rightarrow \infty$  and by the law of large numbers one would expect the evolution to be approximated by the Hamiltonian  $-\Delta + bW$  where  $b = \int V(x)dx$ . Actually, this formal computation leads to the wrong coupling constant. Indeed, the correct limiting Hamiltonian turns out to be

$$(3) \quad H = -\Delta + aW$$

where the constant  $a$  is the scattering length of the unscaled potential  $V$  defined by  $4\pi a = \int V(x)f(x)dx$  where  $f$  is the solution of

$$(-\Delta + V)f = 0$$

with boundary condition  $\lim_{|x| \rightarrow \infty} f(x) = 1$ . Finiteness of  $a$  is guaranteed under the assumption that 0 is neither an eigenvalue nor a resonance for  $V$ . Thus, in the limit of a large number of obstacles the system is described by an Hamiltonian whose only dependence on the interaction potential is through its scattering length, which is indeed known to be the correct parameter describing the interaction in the regime of low energy. We stress that the appearance of the scattering length seems to be in agreement with the more difficult many-body problem where  $N$  particles interact through two-body Gross-Pitaevskii potentials extensively studied, in particular, in the context of Bose-Einstein condensation (see, e.g. [4, 5, 6, 7, 3, 2, 12, 11]).

The convergence of the  $N$  dependent Hamiltonian (2) toward the limiting Hamiltonian (3) is shown in probability in the strong resolvent sense (which in particular implies convergence of the dynamics) and we are also able to characterize fluctuations around the limiting Hamiltonian. For the precise statements of our results we refer to [1, Theorem 1,2]. Remarkably, we don't require positiveness of the potential and negative scattering length are also admissible. The proof is strongly based on the analogy with the study of boundary value problems for the Laplacian on randomly perforated domains addressed in [14, 13, 8, 9, 10] and Hamiltonians with infinitely many point interactions considered in [7].

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**Non-Equilibrium steady states for a thermostatted Lorentz model**

ERIC CARLEN

(joint work with R. Esposito, R. Marra, C. Mouhot and J. Lebowitz)

Consider a particle model for a gas of particles on the one-dimensional torus that interact only through binary energy conserving collisions. We also suppose that there are two types of scatterers distributed on the torus according to some Poisson distribution, as in a Lorentz model, except that each scatterer has a temperature,  $T_1$  or  $T_2$  depending on its type, and a certain radius of interaction, so that when a gas particle travels across the interaction interval, a Poisson clock runs, and if it goes off, the particle assumes a new velocity chosen at random according to the Maxwellian distribution for the temperature of the scatterer.

In an appropriate scaling limit, the net effect of the background scatterers is to produce two uniform thermal reservoirs. Whatever the speed of a gas particle, its

rate of interaction with the reservoirs depends only on the density of the scatterers, again in an appropriate limit in which their intervals of interaction are unlikely to overlap. The kinetic equation that one would expect to arise from such a model in such a limit would be of the type

$$\partial_t f + v\partial_x f = \alpha \mathcal{M}_f + (1 - \alpha)\rho_f \frac{1}{2} (M_{T_1} + M_{T_2}) - f$$

where  $\alpha \in [0, 1]$ ,  $f = f(t, x, v)$ , and

$$M_{T_i}(v) := \frac{e^{-|v|^2 2T_i}}{\sqrt{2\pi T_i}}, \quad \mathcal{M}_f(t, x, v) := \rho_f(t, x) \frac{e^{-\frac{|v|^2}{2T_f(t, x)}}}{\sqrt{2\pi T_f(t, x)}}.$$

except that one might expect a Kac-Povzner type collision kernel, also known as a “soft-spheres” kernel. Our work concerns the kinetic equation itself, and not its rigorous derivation from an underlying particle system, although the brief description of such a system that we have given hopefully illuminates the physical context of our model.

We are concerned with the existence and uniqueness of non-equilibrium steady states (NESS) for our system. It is easy to see that the unique *spatially homogeneous* steady state is given by

$$f_\infty := \alpha M_{T_\infty} + (1 - \alpha) \frac{M_{T_1} + M_{T_2}}{2}, \quad T_\infty = \frac{1}{2}(T_1 + T_2)$$

**Theorem** *For all  $T_1, T_2$ , there is an explicitly computable  $\alpha_0 > 0$  such that for all  $\alpha \in [0, \alpha_0)$ , every steady state solution  $f_\infty$  that belongs to  $L^1(T \times R)$ , has finite second moment and is such that  $\rho \in L^p(T)$  for some  $p > 1$ , is constant in  $x$ .*

We also prove the stability under perturbation for all  $\alpha \in [0, 1]$ . For this, we introduce the (real) Hilbert Space  $\mathcal{H}_\alpha^1$  with inner product

$$\langle f, g \rangle_{\mathcal{H}_\alpha^1} = \int_{T \times R} (f(x, v)(1 - \partial_x^2)g(x, v)) \frac{1}{f_{\alpha, \infty}} dx dv .$$

**Theorem** *For all  $\alpha \in [0, 1]$ , the spatially homogeneous steady state described above is asymptotically stable under perturbation in  $\mathcal{H}_\alpha^1$ . Small perturbations decay exponentially fast in time in this space.*

The theorem shows that if for some  $\alpha > \alpha_0$  there do exist non-uniform steady states, they do not arise as a branch bifurcating off the family of spatially homogeneous steady state solutions.

If  $\alpha = 0$ , the term  $\mathcal{M}_f$  is not present, the only spatially homogeneous steady state is  $f_\infty = \frac{1}{2}(M_{T_1} + M_{T_2})$ , and the equation is linear. It can be interpreted as the forward equation of a Markov process probabilistic methods can-be used to prove that this steady state is unique and is approached exponentially fast. Hence, for  $\alpha = 0$ , there are no steady states that are spatially inhomogeneous.

Next, consider the case  $\alpha = 1$ : there are no thermal reservoirs and energy is conserved. There is a one-parameter infinite family of steady states, namely  $M_T$

for all  $T > 0$ . Moreover, if  $f_0$  is such that

$$\int_{T \times R} v^2 f_0(x, v) dx dv = T, \quad \int_{T \times R} f_0(x, v) \ln f_0(x, v) dx dv < +\infty,$$

and  $f(t, x, v)$  is the solution of with initial datum  $f_0$ , then

$$H(f(t, \cdot, \cdot) | M_T) = \int_{T \times R} f(t, x, v) \ln \frac{f(t, x, v)}{M_T(v)} dx dv$$

decreases monotonically to zero, and is stationary only when  $f = M_T$ . It follows that  $M_T$  is the unique steady state among solutions with second moment equal to  $T$  and finite entropy, and thus every steady state for  $\alpha = 1$  with finite second moment and entropy is spatially homogeneous (and equal to  $M_T$ ).

The rigorous study of NESS for nonlinear kinetic equations remains very challenging. One problem that has been studied by several authors is the Boltzmann equation in a slab with different temperatures on the two walls, with and without external forces. At this level of generality, one cannot always expect a unique NESS – there may be a symmetry breaking transition, such as the onset of Rayleigh-Bernard flow. Even without external forces, existence of NESS for the slab problem is a highly non-trivial, and existing results do not yield provide any information on uniqueness or non-uniqueness. The results obtained here are the only non-perturbative results on this problem that we are aware of.

## The Entropy Problem for the Kac Model

MARIA CARVALHO

(joint work with E. Carlen and A. Einav)

The Entropy Problem for the Kac Model has been actively studied in recent years. We present some new results and discuss some of the remaining problems. This is joint work with E. Carlen and A. Einav.

The Kac Walk is a Markov jump process for an  $N$  particle model of a gas interacting through binary collisions between molecules. At random times arriving in a Poisson stream, pairs of indistinguishable particles, with one clock for each pair, undergo an energy conserving collision in which their velocities are rotated at a random angle, again, chosen uniformly. In a more physically realistic version, the Poisson clocks governing the collision times for pairs of particles could run at rates that are related to the energy of these pairs of particles. In the original model by Kac in 1956 these rates were uniform.

More precisely, the Kac Walk is a continuous time Markov jump process whose state space is  $\mathcal{S}$ , the sphere of radius  $\sqrt{N}$  in  $R^N$ . Let  $\mathbf{v} = (v_1, \dots, v_N)$  denote a generic element of the state-space. The generator  $\mathcal{L}_{N,\gamma}$ , acting on continuous functions  $F$  on  $\mathcal{S}$ , is given by

$$\mathcal{L}_{N,\gamma} F(\mathbf{v}) = -N \binom{N}{2}^{-1} \sum_{i < j} (1 + v_i^2 + v_j^2)^\gamma \frac{1}{2\pi} \int_{-\pi}^{\pi} (F(\mathbf{v}) - F(R_{i,j,\theta} \mathbf{v})) d\theta$$

where  $(R_{i,j,\theta}\mathbf{v})_k = v_i(\theta) = v_i \cos \theta + v_j \sin \theta$  for  $k = i$ , and equals  $v_j(\theta) = -v_i \sin \theta + v_j \cos \theta$  for  $k = j$  and equals  $v_k$  otherwise, and where  $\gamma \in [0, 1]$  is the parameter that measures the relation of the Poisson clocks and the energy of the colliding pair of particles. Let  $d\sigma_N$  denote the uniform probability measure on  $\mathcal{S}$ . It is the unique invariant measure for this process, which is ergodic and reversible. Therefore, the *Kac Master equation*,

$$\frac{\partial}{\partial t} F(\mathbf{v}, t) = \mathcal{L}_{N,\gamma} F(\mathbf{v}, t) ,$$

is the forward Kolmogorov equation describing the evolution of the law  $F(\mathbf{v}, t)d\sigma_N$  of the state under the process (assuming that the law of the initial state is absolutely continuous with respect to  $d\sigma_N$ .) The purpose of Kac's model was to give a probabilistic description of a  $N$  particle gas from which he could deduce, in the limit  $N \rightarrow \infty$ , the evolution of the single particle marginals of solutions of the Kac Master equation with 'chaotic' initial data, by a one dimensional Boltzmann-like equation

$$\frac{\partial}{\partial t} f(v, t) = \mathcal{Q}_\gamma f(v, t)$$

where the non-linear operator  $\mathcal{Q}_\gamma$  is given below. (In his 1956 paper, Kac only consider the case  $\gamma = 0$ , but more recent work has extended his results to other values of  $\gamma$  as discussed below.)

Kac proposed that this rigorous connection between the Master equation and the non-linear Kac-Boltzmann equation could be exploited to prove results on the non-linear evolution equation via analysis of the Kac Walk. He was particularly interested in rates of approach to equilibration. Some recent work on the Kac program has gone in the opposite direction. While the rigorous mathematical investigation of non-linear kinetic equations such as was in a primitive state in 1956 when Kac made his proposal, with most of what was known contained in a 1932 paper of Carleman, it has advanced considerably since that time. A recent paper of Mischler and Mouhot entitled *On Kac's program in kinetic theory* uses the analytic advances in the understanding of the non-linear Boltzmann equation to obtain deep results on the behavior of the Kac Walk.

In this work, we validate Kac's original vision for his program by giving direct proofs of some new functional inequalities for the Kac Walk from which we deduce bounds on the rates of relaxation to equilibrium for solutions of the Kac-Boltzmann equation, just as Kac had proposed. The results we obtain for the Kac Walk themselves are new and interesting, and can be viewed as a partial positive resolution of the 'Almost' Cercignani Conjecture for the Kac Walk, as discussed by Villani. The key to our approach is the introduction of a new strong form of Kac's notion of *chaos*, and we shown that (1) under the assumption of such chaos, there is rapid approach to equilibrium of the 'Almost' Cercignani Conjecture type, and that (2) the chaotic state formed by restricted tensor products satisfy this stronger form of chaos. From these results we deduce 'Almost' Cercignani Conjecture bounds for the Kac-Boltzmann equation.

## A microscopic approach to quadratic cross diffusion systems

LAURENT DESVILLETES

Cross diffusion models are ubiquitous in population dynamics as well as physics. One of the most famous models was proposed by Shigesada, Kawasaki and Teramoto in 1979, cf. [7]. It describes two populations in competition, in which the individuals of one of the populations try to avoid the individuals of the other population, by increasing their diffusion rate in presence of those individuals.

The equations for the densities of the two populations  $u_1 := u_1(t, x)$  and  $u_2 := u_2(t, x)$ , write:

$$\partial_t u_1 - \Delta_x \left( u_1 \left[ D_1 + A_{12} u_2 \right] \right) = (r_1 - S_{11} u_1 - S_{12} u_2) u_1,$$

$$\partial_t u_2 - \Delta_x \left( u_2 \left[ D_2 + A_{21} u_1 \right] \right) = (r_2 - S_{21} u_1 - S_{22} u_2) u_2,$$

where  $D_i, A_{ij}$  are diffusion rates, and  $r_i, S_{ij}$  are coefficients related to the births and deaths of the individuals, taking into account the competition.

Neumann boundary conditions on the boundary of the domain  $\Omega$  can be added to this system: (for  $t \geq 0, x \in \partial\Omega$ )

$$\nabla_x u_1(t, x) \cdot n(x) = 0, \quad \nabla_x u_2(t, x) \cdot n(x) = 0.$$

The study of existence of solutions for this system started with the use of general methods such as those appearing in [1], leading to local strong solutions, and was transformed by the observation, due to Chen and Jüngel (cf. [2]), that the functional

$$J(u_1, u_2) = A_{21} \int_{\Omega} (u_1 \ln u_1 - u_1 + 1) + A_{12} \int_{\Omega} (u_2 \ln u_2 - u_2 + 1)$$

satisfies the following inequality:

$$\begin{aligned} \frac{d}{dt} J(u_1, u_2) + A_{21} D_1 \int \frac{|\nabla_x u_1|^2}{u_1} - A_{12} D_2 \int \frac{|\nabla_x u_2|^2}{u_2} \\ + A_{12} A_{21} \int u_1 u_2 \left| \frac{\nabla_x u_1}{u_1} + \frac{\nabla_x u_2}{u_2} \right|^2 \leq C(r_i, S_{ij}, A_{ij}), \end{aligned}$$

where  $C(r_i, S_{ij}, A_{ij}) > 0$  is a constant. After integration in time, we get indeed that for any  $T > 0$ ,

$$\int_0^T \int_{\Omega} \left( |\nabla_x \sqrt{u_1}|^2 + |\nabla_x \sqrt{u_2}|^2 \right) < \infty,$$

so that compactness can be obtained for  $u_1$  and  $u_2$  (thanks to some variant of Aubin-Lions' lemma), leading first to weak stability of the system, and then, as announced, to existence of global weak solutions in any dimension.

This entropy-like structure can be found in many variants of the Shigesada-Kawasaki-Teramoto system, such as the system (cf. [6]):

$$\begin{aligned} \partial_t u_1 - \Delta_x \left[ (D_1 + A_{12} u_2^{\alpha_{12}}) u_1 \right] &= u_1 \left( r_1 - S_{11} u_1^{\beta_{11}} - S_{12} u_2^{\beta_{12}} \right), \\ \partial_t u_2 - \Delta_x \left[ (D_2 + A_{21} u_1^{\alpha_{21}}) u_2 \right] &= u_2 \left( r_2 - S_{21} u_1^{\beta_{21}} - S_{22} u_2^{\beta_{22}} \right), \end{aligned}$$

when  $0 < \alpha_{12} \alpha_{21} < 1$ , and  $0 < \beta_{ij} < 1$ .

Attempts to explain the appearance of such an entropy-like structure have been made by using microscopic models which converge in some limit to the system of PDEs, and which are naturally endowed with an entropy. They can be larger systems of PDEs depending on a small parameter (related to the time scales), we refer for example to [5] for such a situation. We present here a different approach based on microscopic models which are simple Markov processes. It was observed by Chen, Daus and Jünger (cf. [3]) that the Shigesada-Kawasaki-Teramoto system for an arbitrary number of species, defined as (for  $i = 1, \dots, n$ ):

$$\partial_t u_i = \Delta_x \left( \left[ D_i + \sum_{j=1}^n A_{ij} u_j \right] u_i \right),$$

together with Neumann boundary conditions, is related to the entropy

$$J(u_1, \dots, u_n) := \sum_{i=1}^n \int \pi_i [u_i \ln(u_i) - u_i + 1],$$

as soon as the following condition holds:

$$\forall i, j \quad \pi_i A_{ij} = \pi_j A_{ji}.$$

The system is then said to be detailed balanced.

The corresponding Markov process that we introduced in [4] uses a discretized space domain:  $\Omega_M = \{0, \frac{1}{M}, \frac{2}{M}, \dots, 1\}$ , and nonnegative constants  $\pi_i, D_i, D_{ij}$  such that  $\sum_{i=1}^n \pi_i = 1$  and  $D_{ij} = D_{ji}$  for  $i, j = 1, \dots, n$ . We consider  $n$  species of particles located on  $\Omega_M$ . Then we consider  $[\pi_i N]$  particles of species  $i$ , and introduce the time-continuous Markov chain on  $\Theta_{M,N} := \Omega_M^{[\pi_1 N] + \dots + [\pi_n N]}$  by the transitions

$$\begin{aligned} \left. \begin{aligned} x &\rightarrow x + e_i^a + e_j^b \\ x &\rightarrow x - e_i^a - e_j^b \end{aligned} \right\} && \text{with rate } \delta_{(i,a) \neq (j,b)} \delta_{x_i^a = x_j^b} \frac{D_{ij}}{N} \\ \left. \begin{aligned} x &\rightarrow x + e_i^a \\ x &\rightarrow x - e_i^a \end{aligned} \right\} && \text{with rate } D_i \end{aligned}$$

for  $i, j = 1, \dots, n$  and  $a = 1, \dots, [\pi_i N], b = 1, \dots, [\pi_j N]$ , where  $e_i^a$  is the vector with components of value zero at all places, except for the  $a$ -th particle of species  $i$ , where the value is  $h = 1/M$ .

We show that the functional defined by

$$\tilde{\mathcal{H}}(\mu^N)(t) := \sum_x \mu^N(t, x) \ln \left( \frac{\mu^N(t, x)}{M^{[\pi_1 N] + \dots + [\pi_n N]}} \right)$$

is decreasing with respect to time.

When  $N \rightarrow \infty$ , under the assumption (of indistinguishability and) chaos propagation:

$$\begin{aligned} & \mu^N(t, x_1^1, \dots, x_1^{[\pi_1 N]}, \dots, x_n^1, \dots, x_n^{[\pi_n N]}) \\ & \approx u_1(t, x_1^1) \cdots u_1(t, x_1^{[\pi_1 N]}) \cdots u_n(t, x_n^1) \cdots u_n(t, x_n^{[\pi_n N]}), \end{aligned}$$

one can show that

$$\begin{aligned} \frac{d}{dt} u_i(t, x) &= D_i \left[ u_i(t, x+h) + u_i(t, x-h) - 2u_i(t, x) \right] \\ &+ \sum_{j=1}^n D_{ij} \pi_j \left[ u_j(t, x+h) u_i(t, x+h) + u_j(t, x-h) u_i(t, x-h) - 2u_j(t, x) u_i(t, x) \right]. \end{aligned}$$

and

$$\begin{aligned} \frac{1}{N} \tilde{\mathcal{H}}(\mu^N) &= \sum_x \mu^N(x) \ln \left( \frac{\mu^N(x)}{M^{([\pi_1 N] + \dots + [\pi_n N])}} \right) \\ &\approx \frac{1}{N} \sum_{i=1}^n \sum_{\ell=0}^{M-1} [\pi_i N] u_i(x_\ell) \ln \left( \frac{u_i(x_\ell)}{M} \right) \\ &\rightarrow \sum_{i=1}^n \pi_i \sum_{\ell=0}^{M-1} u_i(x_\ell) \ln \left( \frac{u_i(x_\ell)}{M} \right). \end{aligned}$$

When  $h = 1/M \rightarrow 0$ , defining  $A_{ij} := \pi_j D_{ij}$ , and rescaling in time (in such a way that  $\partial_t$  is replaced by  $h^2 \partial_t$ ), one recovers the original Shigesada-Teramoto-Kawasaki system for an arbitrary number of species, and its entropy-like functional

$$J(u_1, \dots, u_n) := \sum_{i=1}^n \int \pi_i [u_i \ln(u_i) - u_i + 1].$$

The condition  $\forall i, j \ D_{ij} = D_{ji}$  then becomes the detailed balance condition.

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## Empirical Measures and Quantum Dynamics

FRANÇOIS GOLSE

(joint work with Thierry Paul)

**1. Introduction.** A remarkable feature of the classical mechanics of systems of  $N$  identical point particles is the notion of Klimontovich solutions of the Vlasov equation, recalled below. Let  $V \in C^{1,1}(\mathbf{R}^d)$  be an even function. For each  $N \geq 2$ , and each  $Z_N := (z_1, \dots, z_N) \in (\mathbf{R}^{2d})^N$ , set

$$\mu_{Z_N} := \frac{1}{N} \sum_{j=1}^N \delta_{z_j}.$$

**Klimontovich's Theorem** *Let  $t \mapsto Z_N(t)$  be a  $C^1$   $N$ -particle trajectory. Then  $t \mapsto \mu_{Z_N(t)}$  is a weak solution to the Vlasov equation*

$$(1) \quad \left( \partial_t + \frac{1}{m} \xi \cdot \nabla_x \right) f(t, x, \xi) - \nabla_x V_f(t, x) \cdot \nabla_\xi f(t, x, \xi) = 0,$$

where

$$V_f(t, x) := \iint_{\mathbf{R}^{2d}} V(x - y) f(t, y, \eta) dy d\eta,$$

if and only if  $z_j(t) = (q_j(t), p_j(t))$  is a solution to the system of Newton's 2nd law written for each particle (with  $m$  denoting the mass of each particle)

$$(2) \quad \dot{q}_j = \frac{1}{m} p_j, \quad \dot{p}_j = -\frac{1}{N} \sum_{k=1}^N \nabla V(q_j(t) - q_k(t)), \quad j = 1, \dots, N.$$

The proof of this result is elementary if one observe that  $\dot{p}_j(t) = -\nabla_x V_\mu(t, q_j(t))$ , so that (2) is the equivalent to the defining equations for characteristic curves of the Vlasov equation. With this observation, deriving the Vlasov equation from the dynamics of  $N$ -particle systems amounts to proving the continuous dependence of the solution of the Vlasov equation on its initial data for the weak topology of Borel probability measures on  $\mathbf{R}^{2d}$ . This has been done in [1, 2]. Whether an analogue of the Klimontovich theorem exists in quantum dynamics has been an open question<sup>1</sup> since the work of Braun-Hepp [1].

**2. A Quantum Notion of Empirical Measure.** Denote by  $T_t^N$  the flow generated by the differential system (2). Let  $F_N^{in} \equiv F_N^{in}(z_1, \dots, z_N)$  be a symmetric

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<sup>1</sup>We thank Mario Pulvirenti for introducing us to that problem.

probability density on  $(\mathbf{R}^{2d})^N$ , and set  $F_N(t, Z_N) := F_N^{in}(T_{-t}^N Z_N)$ . Then  $F_N(t, \cdot)$  is also a symmetric function of the variables  $z_j$  and one has

$$(3) \quad \int_{(\mathbf{R}^{2d})^N} \langle \mu_{T_t^N Z_N}, \phi \rangle F_N^{in}(Z_N) dZ_N = \int_{\mathbf{R}^{2d}} \phi(x, \xi) F_{N:1}(t, x, \xi) dx d\xi$$

for all  $\phi \in C_b(\mathbf{R}^{2d})$ , where  $F_{N:1}$  is the first marginal of  $F_N$ , defined by the formula

$$F_{N:1}(t, z) := \int_{(\mathbf{R}^{2d})^{N-1}} F_N(t, z, z_2, \dots, z_N) dz_2 \dots dz_N, \quad z = (x, \xi) \in \mathbf{R}^{2d}.$$

This follows for instance from Theorem 3.1 (a) in [4].

Our definition of the quantum analogue of the notion of empirical measure is based on (3). Denote  $\mathfrak{H} := L^2(\mathbf{R}^d)$  and  $\mathfrak{H}_N := \mathfrak{H}^{\otimes N} \simeq L^2(\mathbf{R}^{Nd})$ , and define the set of density operators on  $\mathfrak{H}$  as

$$\mathcal{D}(\mathfrak{H}) := \{R \in \mathcal{L}(\mathfrak{H}) \text{ s.t. } R = R^* \geq 0 \text{ and } \text{trace}(R) = 1\}.$$

For each permutation  $\sigma \in \mathfrak{S}_N$ , denote by  $U_\sigma$  the operator defined on  $\mathfrak{H}_N$  by

$$U_\sigma \Psi_N(x_1, \dots, x_N) := \Psi_N(x_{\sigma^{-1}(1)}, \dots, x_{\sigma^{-1}(N)}).$$

An operator  $T \in \mathcal{L}(\mathfrak{H}_N)$  is said to be symmetric if  $U_\sigma S U_\sigma^* = S$  for all  $\sigma \in \mathfrak{S}_N$ . One denote by  $\mathcal{L}_s(\mathfrak{H}_N)$  the set of symmetric bounded operators on  $\mathfrak{H}_N$ , by  $\mathcal{L}_s^1(\mathfrak{H}_N) := \mathcal{L}^1(\mathfrak{H}_N) \cap \mathcal{L}_s(\mathfrak{H}_N)$  and  $\mathcal{D}_s(\mathfrak{H}_N) := \mathcal{D}(\mathfrak{H}_N) \cap \mathcal{L}_s(\mathfrak{H}_N)$  (the sets of symmetric trace-class operators and of symmetric density operators on  $\mathfrak{H}_N$ ). For all  $T \in \mathcal{L}_s^1(\mathfrak{H}_N)$ , one denotes by  $T_{:1}$  its partial trace defined by

$$\text{trace}_{\mathfrak{H}}(AT_{:1}) = \text{trace}_{\mathfrak{H}_N}((A \otimes I_{\mathfrak{H}_{N-1}})T), \quad \text{for each } A \in \mathcal{L}(\mathfrak{H}).$$

Finally, the quantum dynamics is defined in terms of the quantum Hamiltonian

$$\mathcal{H}_N := -\frac{1}{2m} \hbar \sum_{j=1}^N \Delta_{x_j} + \frac{1}{N} \sum_{1 \leq j < k \leq N} V(x_j - x_k),$$

which has an unbounded self-adjoint extension on  $\mathfrak{H}_N$  for  $V \in L^\infty(\mathbf{R}^d)$ .

**Definition.** The quantum Klimontovich density evolved along the quantum dynamics defined by  $\mathcal{H}_N$  is the adjoint, denoted  $\mathcal{M}_N(t)$ , of the linear map

$$\mathcal{L}_s^1(\mathfrak{H}_N)T \mapsto \left( e^{-it\mathcal{H}_N/\hbar} T e^{+it\mathcal{H}_N/\hbar} \right)_{:1} \in \mathcal{L}^1(\mathfrak{H}).$$

In other words, for each  $A \in \mathcal{L}(\mathfrak{H})$ , the quantum analogue of the identity (3) is

$$(4) \quad \text{trace}_{\mathfrak{H}_N}((\mathcal{M}_N(t)A)T) = \text{trace}_{\mathfrak{H}} \left( A \left( e^{-it\mathcal{H}_N/\hbar} T e^{+it\mathcal{H}_N/\hbar} \right)_{:1} \right).$$

One easily checks that, for each  $A \in \mathcal{L}(\mathfrak{H})$  and each  $t \geq 0$ , one has

$$\mathcal{M}_N(t)A = e^{+it\mathcal{H}_N/\hbar} (\mathcal{M}_N(0)A) e^{-it\mathcal{H}_N/\hbar},$$

and that

$$\mathcal{M}_N(0) = \frac{1}{N} \sum_{k=1}^N J_k, \quad \text{where } J_k A := I_{\mathfrak{H}}^{\otimes(k-1)} \otimes A \otimes I_{\mathfrak{H}}^{\otimes(N-k)}.$$

**3. An Equation for  $\mathcal{M}_N(t)$ .** That there is a “closed” equation satisfied by  $\mathcal{M}_N(t)$  is not obvious a priori, since there is no closed equation for the first marginal of the solution of the  $N$ -particle von Neumann equation — this is the reason for considering the BBGKY hierarchy when dealing with  $N$ -particle systems in quantum mechanics.

**Theorem A.** [5] Denoting by  $\mathcal{F}$  the Fourier transformation, let  $V \in \mathcal{FL}^1(\mathbf{R}^d)$  be a real-valued even function. Then  $\mathcal{M}_N(t)$  is a weak solution of

$$(5) \quad i\hbar\partial_t\mathcal{M}_N(t) = \mathbf{ad}^*\left(-\frac{1}{2m}\hbar^2\Delta\right)\mathcal{M}_N(t) - \mathcal{C}[V, \mathcal{M}_N(t), \mathcal{M}_N(t)],$$

where, for each  $\Lambda \in \mathcal{L}(\mathfrak{H}), \mathcal{L}_s(\mathfrak{H}_n)$  and each unbounded operator  $H$  on  $\mathfrak{H}$ ,

$$(\mathbf{ad}^*(H)\Lambda)A := -\Lambda([H, A]) \text{ for each } A \in \mathcal{L}(\mathfrak{H}) \text{ such that } [H, A] \in \mathcal{L}(\mathfrak{H}),$$

while, denoting  $E_\omega$  the operator on  $\mathfrak{H}$  defined by  $E_\omega\psi(x) = e^{i\omega\cdot x}\psi(x)$ ,

$$\mathcal{C}[V, \Lambda, \Lambda]A := \int_{\mathbf{R}^d} (\Lambda(E_\omega^*)\Lambda(E_\omega A) - \Lambda(AE_\omega)\Lambda(E_\omega^*))\mathcal{F}V(\omega)\frac{d\omega}{(2\pi)^d}.$$

At variance with the case of classical mechanics, (5) does not coincide with the Hartree equation (which is the quantum analogue of the Vlasov equation). However, it contains the Hartree equation as explained below.

**Theorem B.** [5] Denote by  $\mathcal{R}_N(t)$  the time-dependent element of  $\mathcal{L}(\mathcal{L}(\mathfrak{H}), \mathcal{L}_s(\mathfrak{H}_n))$  defined by

$$\mathcal{R}_N(t) := \text{trace}(AR(t))I_{\mathfrak{H}_N},$$

where  $t \mapsto R(t)$  is a continuous time-dependent density operator on  $\mathfrak{H}$ . Then  $\mathcal{R}_N$  is a weak solution of (5) if and only if  $R$  is a weak solution to the Hartree equation

$$i\hbar\partial_t R(t) = \left[-\frac{1}{2m}\hbar^2\Delta + V_{R(t)}, R(t)\right], \quad V_{R(t)}(x) := \text{trace}_{\mathfrak{H}}(V(x - \cdot)R(t)).$$

**4. Application to the Mean-Field Limit in Quantum Mechanics.** Assume further that  $\mathbf{V} := \|(1 + |\xi|)^{[d/2]+3}\mathcal{F}V\|_{L^1(\mathbf{R}^d)} < \infty$  and set

$$\Psi_{N,\hbar}(t, x_1, \dots, x_N) := e^{-it\mathcal{H}_N/\hbar} \prod_{k=1}^n \psi_{\hbar}^{in}(x_k), \quad \text{with } \|\psi_{\hbar}^{in}\|_{L^2(\mathbf{R}^d)} = 1,$$

while  $\psi_{\hbar} \equiv \psi_{\hbar}(t, x)$  is the solution of

$$i\hbar\partial_t\psi_{\hbar}(t, x) = \left(-\frac{1}{2m}\hbar^2\Delta_x + V \star |\psi_{\hbar}(t, \cdot)|^2(x)\right)\psi_{\hbar}(t, x), \quad \psi_{\hbar}(0, \cdot) = \psi_{\hbar}^{in}.$$

**Theorem C.** [5] There exists  $C[\mathbf{V}, d] > 0$  such that, for each  $t \geq 0$

$$\|W_{\hbar}[[\Psi_{N,\hbar}]\langle\Psi_{N,\hbar}|_{:1}(t)] - W_{\hbar}[[\psi_{\hbar}]\langle\psi_{\hbar}|(t)]\|'_{[d/2]+2} \leq \frac{C[\mathbf{V}, d]e^{C[\mathbf{V}, d]te^{C[\mathbf{V}, d]}}}{\sqrt{N}},$$

where  $\|\cdot\|'_n$  designates the dual norm of

$$\|\phi\|'_n := \sup \left\{ \int_{\mathbf{R}^{2d}} \phi f(x, \xi) dx d\xi \text{ for all } f \text{ s.t. } \max_{|\alpha|, |\beta| \leq n} \|\partial_x^\alpha \partial_\xi^\beta f\|_{L^\infty(\mathbf{R}^{2d})} \leq 1 \right\},$$

while  $W_{\hbar}[R]$  is the Wigner transform of the density operator  $R$ , defined in terms of the integral kernel  $r$  of  $R$  by the formula (see [8]):

$$W_{\hbar}[R](x, \xi) := \frac{1}{(2\pi)^d} \int_{\mathbf{R}^d} e^{-i\xi \cdot y} r(x + \frac{1}{2}\hbar y, x - \frac{1}{2}\hbar y) dy.$$

Theorem C provides an  $O(1/\sqrt{N})$  convergence rate uniformly in  $\hbar$  for the mean-field limit in the quantum dynamics of  $N$  identical particles interacting via the potential  $V$ . The interest for the uniformity in  $\hbar$  stems for very small size of the Planck constant  $\hbar = 1.1 \cdot 10^{-34} J \cdot s$ . Earlier estimates (see for instance [10, 9]) for the convergence rate in that limit allowed for more singular potentials (including the Coulomb potential) but typically led to a nonuniform in  $\hbar$  control of order  $O(e^{Ct/\hbar}/\sqrt{N})$ . Other approaches to the uniformity in  $\hbar$  of the convergence rate for the mean-field limit in quantum mechanics can be found in [7, 3, 6] — see also the bibliography of [5] for more references on this topic.

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### Quantum Transport in a Low-Density Periodic Potential: Homogenisation via Homogeneous Flows

JORY GRIFFIN

(joint work with J. Marklof)

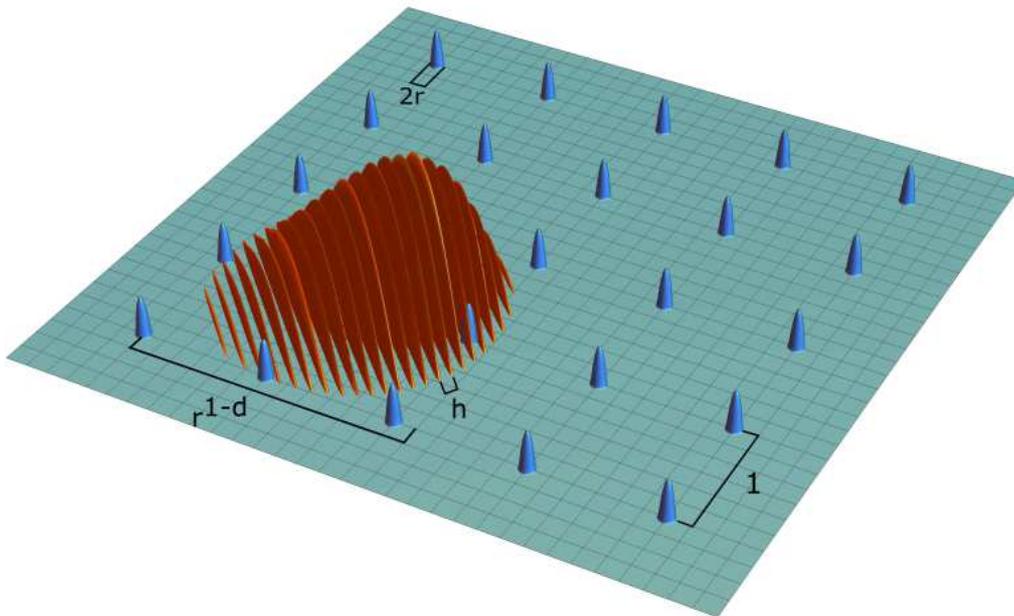
**The Quantum Lorentz Gas** The quantum Lorentz gas consists of an initial wave packet that evolves according to the  $d$ -dimensional Schrödinger equation with potential given by an infinite array of compactly supported profiles placed on the elements of some discrete point set. It is shown by Eng and Erdős [2] that if the scatterers are placed randomly, then the Husimi function converges, in

the Boltzmann-Grad or low-density limit, to a solution of the linear Boltzmann equation

$$(1) \quad \partial_t f(t, x, y) + y \cdot \nabla_x f(t, x, y) = \int \Sigma(y, y') [f(t, x, y') - f(t, x, y)] dy'.$$

This result is directly analogous to those of Gallavotti, Spohn, and Boldrighini-Bunimovich-Sinai [3, 7, 1] for when the underlying dynamics is classical rather than quantum.

Our focus is to investigate the case of scatterers placed on  $\mathbb{Z}^d$ . In words, the main result of our work is that convergence in the Boltzmann-Grad limit occurs in the periodic case, at least up to second order in the coupling constant (i.e. the ‘strength’ of the scatterers). In contrast with the classical case (See e.g. [6]), the limit (up to second order) agrees with the linear Boltzmann equation, although we conjecture disagreement at all orders larger than four.



*Fig. A schematic picture showing a wave packet evolving in a periodic array of scatterers with the relevant scales marked.*

**The Model** Let  $W$  be some smooth function with compact support in the unit ball. Consider the Hamiltonian  $H_{h,\lambda} = -\frac{\hbar^2}{8\pi^2} \Delta + \lambda V$  where

$$(2) \quad V(x) = V_r(x) = \sum_{m \in \mathbb{Z}^d} W\left(\frac{x-m}{r}\right).$$

The Boltzmann-Grad limit corresponds to taking the limit  $r \rightarrow 0$  while simultaneously rescaling space and time. We work in the Heisenberg picture, and assume the initial condition  $\text{Op}(a)$  is the Weyl quantisation of some classical phase space density. At time  $t$  the Heisenberg evolution of  $\text{Op}(a)$  is given by

$$(3) \quad A(t) = U_{h,\lambda}(t) \text{Op}(a) U_{h,\lambda}(-t)$$

where  $U_{h,\lambda}(t) = e(-H_{h,\lambda}t/h)$  and we define  $e(x) = e^{2\pi i x}$ . In order to pass to the Boltzmann-Grad limit we introduce the dilation operator

$$(4) \quad D_{r,h}a(x, y) = r^{d(d-1)/2} h^{d/2} a(r^{d-1}x, hy)$$

and put  $\text{Op}_{r,h}(a) = \text{Op}(D_{r,h}a)$ . The object of interest is then the operator

$$(5) \quad A_r(t) = U_{h,\lambda}(r^{1-d}t) \text{Op}_{r,h}(a) U_{h,\lambda}(-r^{1-d}t) \Big|_{h=r}.$$

The scaling regime  $a \rightarrow D_{r,h}a$  and  $t \rightarrow r^{1-d}t$  is precisely analogous to the Boltzmann-Grad regime in the classical problem, and the choice  $h = r$  is to ensure truly quantum scattering (wavelength is comparable to scatterer size).

**Statement of Results** Convergence is established term-by-term in a formal expansion. Duhamel's principle tells us that

$$(6) \quad U_{h,\lambda}(t) = U_{h,0}(t) - 2\pi i \lambda \int_0^t U_{h,\lambda}(s) \text{Op}(V) U_{h,0}(t-s) ds,$$

which after iterating yields the formal expansion  $A_r(t) = \sum_{n=0}^{\infty} \lambda^n A_r^{(n)}(t)$ . Similarly, if one returns to the linear Boltzmann equation (1), integrates, and expands in  $\lambda$ , one obtains the formal expansion  $f(t, x, y) = \sum_{n=0}^{\infty} \lambda^n f^{(n)}(t, x, y)$ .

**Theorem 1.** For  $a$  and  $b$  smooth and compactly supported and for  $n = 0, 1, 2$  we have

$$\lim_{r=h \rightarrow 0} \langle A_r^{(n)}(t), \text{Op}_{r,h}(b) \rangle_{\text{HS}} = \int_{\mathbb{R}^{2d}} f^{(n)}(t, x, y) b(x, y) dx dy.$$

In fact we prove something stronger than this. Floquet-Bloch theory allows one to decompose the periodic problem on  $\mathbb{R}^d$  into a family of quasiperiodic problems on  $\mathbb{T}^d$  parametrised by  $\alpha$ . We denote the solutions to this family of problems by  $A_{r,\alpha}$  and the terms in their Duhamel expansions by  $A_{r,\alpha}^{(n)}$ . One should think of the  $A_{r,\alpha}$  as being solutions to the problem on the torus, with a single scatterer, and with domains restricted to quasiperiodic functions that satisfy  $f(x+m) = e(m \cdot \alpha) f(x)$  for  $m \in \mathbb{Z}^d$ .

**Theorem 2.** Let  $\alpha$  satisfy an explicit Diophantine condition. Then, for  $a$  and  $b$  smooth and compactly supported and for  $n = 0, 1, 2$  we have

$$\lim_{r=h \rightarrow 0} \langle A_{r,\alpha}^{(n)}(t), \text{Op}_{r,h}(b) \rangle_{\text{HS}} = \int_{\mathbb{R}^{2d}} f^{(n)}(t, x, y) b(x, y) dx dy.$$

The terms at orders zero and one converge using standard techniques so we focus on order two. The approach will be to prove Theorem 2 first, and then Theorem

1 will follow by integrating over  $\alpha$  and applying some dominated convergence estimates.

**Homogeneous Dynamics** Consider the semi-direct product group  $G = \text{SL}(2, \mathbb{R}) \ltimes \mathbb{R}^{2d}$  with multiplication law

$$(7) \quad (M, \xi)(M', \xi') = (MM', \xi + M\xi'),$$

where  $M, M' \in \text{SL}(2, \mathbb{R})$ ,  $\xi, \xi' \in \mathbb{R}^d \times \mathbb{R}^d$  and the product  $M\xi$  is defined via the embedding  $\begin{pmatrix} a & b \\ c & d \end{pmatrix} \mapsto \begin{pmatrix} aI & bI \\ cI & dI \end{pmatrix}$ .

It is well known that one can associate  $\text{SL}(2, \mathbb{R})$  with the unit tangent bundle of the complex upper half plane  $\mathfrak{H} = \{\tau \in \mathbb{C} : \Im\tau > 0\}$  via the Iwasawa decomposition

$$(8) \quad M = \begin{pmatrix} 1 & u \\ 0 & 1 \end{pmatrix} \begin{pmatrix} v^{1/2} & 0 \\ 0 & v^{-1/2} \end{pmatrix} \begin{pmatrix} \cos \phi & -\sin \phi \\ \sin \phi & \cos \phi \end{pmatrix}.$$

We can thus use the notation  $(M, \xi)$  or  $(\tau, \phi, \xi)$  interchangeably. In the following,  $\Gamma$  is a subgroup of  $\text{SL}(2, \mathbb{Z}) \ltimes (\frac{1}{2}\mathbb{Z})^{2d}$  of finite index. In this case the quotient  $\Gamma \backslash G$  is a non-compact manifold with finite volume with respect to the Haar measure  $\mu$ .

**Proposition 1** (Marklof [5]). Fix  $y \in \mathbb{R}^d \setminus \mathbb{Q}^d$  so that the components of  $(1, y^t)$  are linearly independent over  $\mathbb{Q}$ . Let  $w : \mathbb{R} \rightarrow \mathbb{R}$  piecewise continuous with compact support. Let  $F : \Gamma \backslash G \rightarrow \mathbb{R}$  be bounded continuous. Then for all  $\sigma \geq 0$  we have

$$\lim_{v \rightarrow 0} v^\sigma \int_{\mathbb{R}} F((u + iv, 0, \begin{pmatrix} 0 \\ y \end{pmatrix})) w(v^\sigma u) du = \frac{1}{\mu(\Gamma \backslash G)} \int_{\Gamma \backslash G} F d\mu \int_{\mathbb{R}} w(u) du.$$

Let us explain this proposition intuitively. We are computing the average of some ‘nice’ function  $F$  over a curve (in fact a piece of a *horocycle*) parametrised by  $v^\sigma u \in \text{supp } w$ . The curve sits at height  $v$  in the complex upper half plane, and in the limit  $v \rightarrow 0$ , due to the hyperbolic geometry and the fact that  $\sigma \geq 0$ , it gets longer and longer. This proposition tells us that eventually this long segment becomes equidistributed on the entire manifold, so the one dimensional average of  $F$  can be replaced by the  $\mu$  average.

**Proposition 2.** There exists an explicit subgroup  $\Gamma$  and an explicit convergent sequence of  $C^\infty$  functions  $(F_r)_{r \geq 0} : \Gamma \backslash G \times \mathbb{R} \rightarrow \mathbb{C}$  such that

$$(9) \quad \langle A_{r,\alpha}^{(2)}(t), \text{Op}_{r,r}(b) \rangle_{\text{HS}} = r^{d-2} \int_{\mathbb{R}} F_r((u + iv, 0, \begin{pmatrix} 0 \\ -\alpha \end{pmatrix}), r^{d-2}u) du + O(r^\infty)$$

Our second order terms can thus be viewed as a nice function on the manifold  $\Gamma \backslash G$  averaged along a curve that becomes equidistributed. Theorem 2 then follows by taking the limit  $r \rightarrow 0$ , computing the  $\mu$  integral, and comparison with  $f^{(2)}$ . To do this we need to generalise Proposition 1 in a few ways. First of all our functions  $F_r$  are not bounded – it is for this reason that one needs some Diophantine condition on  $\alpha$  (see [5]). Secondly, we need to be able to apply Proposition 1 to a *convergent sequence* of functions  $F_r$ , and finally we need to replace  $F(g)w(u)$  by  $F(g, u)$ , that is, we should include functions on the product space  $\Gamma \backslash G \times \mathbb{R}$  which cannot be factorised.

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## Rough paths and the random Schrödinger equation

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Introduced by Lyons in his influential '98 paper [6], *rough paths* have nowadays grown to a very complete theory for the study of controlled differential equations driven by rough signals [2]. One of the key ideas is that of working with description of the functions of interest in terms of *local developments* around an arbitrary point. Rough path theory allows both to parametrise these local developments and also “integrate” them to produce global analytic objects. These features are also at the base of Hairer’s *regularity structures* theory [4].

In this talk we discussed the relevance of these local descriptions in the analysis of the long time behaviour of a random Schrödinger equation. A motivation for this is to have a toy model where to explore the applicability of ideas from rough path theory to the analysis of the kinetic limit of certain systems evolving in random environment like a classical particle colliding with Poissonian obstacles or a quantum particle in a Gaussian random environment (see the work of Gallavotti or Kesten and Papanicolau [5] in the classical case or the work of Erdős and Yau [1] for the kinetic limit in the quantum case).

Consider the following random Schrödinger equation on  $\mathbb{T}^d$ :

$$(1) \quad i\partial_t \varphi(t) = \Delta \varphi(t) + \varepsilon V \varphi(t),$$

where  $V$  is a time-independent centered Gaussian random potential with smooth covariance. The parameter  $\varepsilon$  will be taken to go to zero. Let  $\psi_\varepsilon(t) = e^{it\Delta/\varepsilon} \varphi(t/\varepsilon^2)$  then  $i\partial_t \psi_\varepsilon(t) = \varepsilon^{-1} e^{it\Delta/\varepsilon^2} V e^{-it\Delta/\varepsilon^2} \psi_\varepsilon(t)$  and by expanding the solution around an arbitrary point  $s$  we get

$$(2) \quad \psi_\varepsilon(t) = \psi_\varepsilon(s) + \mathbb{X}_{s,t}^{1,\varepsilon} \psi_\varepsilon(s) + \mathbb{X}_{s,t}^{2,\varepsilon} \psi_\varepsilon(s) + o(|t - s|)$$

where we introduced the random operators

$$\mathbb{X}_{s,t}^{1,\varepsilon} = -\frac{i}{\varepsilon} \int_s^t e^{ir\Delta/\varepsilon^2} V e^{-ir\Delta/\varepsilon^2} dr, \quad \mathbb{X}_{s,t}^{2,\varepsilon} = -\frac{i}{\varepsilon} \int_s^t (e^{ir\Delta/\varepsilon^2} V e^{-ir\Delta/\varepsilon^2}) \mathbb{X}_{s,r}^1 dr,$$

which satisfy the operator Chen relation

$$\mathbb{X}_{s,t}^{2,\varepsilon} = \mathbb{X}_{s,u}^{2,\varepsilon} + \mathbb{X}_{u,t}^{2,\varepsilon} + \mathbb{X}_{u,t}^{1,\varepsilon} \mathbb{X}_{s,u}^{1,\varepsilon}, \quad s \leq u \leq t.$$

The local expansion (2) can be used in the spirit of controlled paths [3] to obtain uniform control on the solution  $\psi$  wrt. the data  $\mathbb{X}^\varepsilon = (\mathbb{X}^{1,\varepsilon}, \mathbb{X}^{2,\varepsilon})$  which can be viewed as a rough path. Some probabilistic estimate allow to control the limit  $\varepsilon \rightarrow 0$  of  $\mathbb{X}^\varepsilon$  (in law) and show that, after a renormalization which removes some resonant terms one has  $\mathbb{X}^{1,\varepsilon} \rightarrow 0$  and  $\mathbb{X}_{s,t}^{2,\varepsilon} \rightarrow (t-s)(-iH)$  for some deterministic operator  $H : L^2 \rightarrow L^2$ . The convergence is in the Hilbert-Schmidt topology wrt.  $L^2(\mathbb{T}^d)$ . As a consequence  $\psi_\varepsilon$  converges to the solution  $\psi$  of the linear equation

$$i\partial_t \psi = H\psi.$$

Unfortunately the need for renormalisation, due to resonances produced by the periodic boundary conditions force to modify eq. (1) adding non-local  $O(1)$  terms and making the problem less natural. A possible way out is to set up the problem in the space of quasi-periodic functions which would allow to remove the bad resonances. It would also be interesting to work in the full space but this causes much trouble in the identification of the suitable topology in which to look for the convergence of the stochastic operators  $\mathbb{X}^\varepsilon$  and we could not yet find a viable approach.

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### Effective dynamics for the Nelson model with many fermions

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(joint work with S. Petrat)

Quantum fields are used in various branches of physics, such as quantum optics, ultra-cold quantum gases and condensed matter physics. The underlying picture is that particles create and annihilate field bosons. This leads to an exchange of energy and creates an interaction between the particles. In the presence of a large number of bosons the action of an individual one is often negligible and the bosons collectively behave like a classical radiation field. To a good extent it is then possible to approximate the evolution of the system by a set of simpler effective

equations in which the quantum field is replaced by a pair potential or a classical field obeying a wave equation. A mathematical justification of this approximation is important because it shows its validity and provides insights into the mechanism that leads to the emergence of classical radiation. In [1, 3, 4, 5, 6, 7, 8, 9, 11, 12] classical field equations were derived from systems in which bosons or a small number of fermions couple to a quantized radiation field. Moreover, it was shown (see [10] for references) that quantum fields can sometimes be approximated by a two-particle interaction if the particles are much slower than the bosons of the radiation field. Our goal is to show the creation of classical radiation in a many particle limit of fermions. We consider  $N$  identical fermions which interact by means of a quantized scalar field. The state of the system is described by a wave function  $\Psi_{N,t} \in L^2_{\text{as}}(\mathbb{R}^{3N}) \otimes \mathcal{F}$ , where "as" indicates antisymmetry under exchange of variables and  $\mathcal{F}$  denotes the bosonic Fock space over  $L^2(\mathbb{R}^3)$ . The time evolution of the system is described by the Schrödinger equation

$$(1) \quad i\partial_t \Psi_{N,t} = N^{-1/3} H_N \Psi_{N,t},$$

where

$$H_N = \sum_{j=1}^N \left( -\Delta_j + \hat{\Phi}_\Lambda(x_j) \right) + \delta_N H_f \quad \text{with} \quad H_f = \int d^3k \omega(k) a^*(k) a(k) \quad \text{and}$$

$$\hat{\Phi}_\Lambda(x) = \int d^3k \frac{1}{\sqrt{16\pi^3\omega(k)}} \mathbb{1}_{|k| \leq \Lambda}(k) \left( e^{ikx} a(k) + e^{-ikx} a^*(k) \right)$$

is the Nelson Hamiltonian with ultraviolet cutoff  $\Lambda$ . We are interested in situations in which the electrons are localized in a volume of order one. The average momentum per fermion is then of order  $N^{1/3}$  because of the Fermi statistics. Thus if we want to monitor the particles while they are moving in the volume of order one, we have to consider time scales of order  $N^{-1/3}$ . This explains the factor  $N^{-1/3}$  in the Schrödinger equation. The dispersion relations of the field bosons is given by  $\omega(k) = \sqrt{|k|^2 + m^2}$  with  $m \geq 0$  and  $\delta_N$  is a  $N$ -dependent parameter. Our main result holds for all  $\delta_N$ . However, we think that the choice  $\delta_N = N^{1/3}$  is the most interesting because it implies that the velocities of the electrons and the field bosons scale equally and that the interaction plays a significant role in the effective evolution equations (4). Also  $\delta_N = 1$  is a good choice as our model then describes an unscaled system whose dynamics is inspected on times of order  $N^{-1/3}$ . In this case the group velocity of the field bosons is too slow to mediate an interaction and the electrons approximately behave like free particles in a stationary external potential (see Theorem II.9 in [10]).

We consider initial states of product form  $\Psi_{N,0} = \bigwedge_{j=1}^N \varphi_j^0 \otimes W(N^{2/3} \alpha^0) \Omega$  where  $\alpha_0 \in L^2(\mathbb{R}^3)$ ,  $\bigwedge_{j=1}^N \varphi_j^0$  is the antisymmetrized product of orthonormal functions  $\varphi_1^0, \dots, \varphi_N^0 \in L^2(\mathbb{R}^3)$ ,  $\Omega$  denotes the vacuum in  $\mathcal{F}$  and  $W$  is the Weyl operator

$$W(f) = \exp \left( \int d^3k f(k) a^*(k) - \overline{f(k)} a(k) \right) \quad \text{for all } f \in L^2(\mathbb{R}^3).$$

To derive our result on the chosen time scale, it is in addition necessary to require (an important fact which we learned from [2]) that the momenta of the electrons are uniformly distributed (first condition in (2)) and that the density of the electrons varies on a scale of order one (second inequality in (2)).

**Assumption 1.** *Let  $\varphi_1^0, \dots, \varphi_N^0 \in H^2(\mathbb{R}^3)$  be orthonormal and such that*

$$(2) \quad \text{Tr} |p^0 e^{ikx} q^0| \leq C(1 + |k|)N^{2/3} \forall k \in \mathbb{R}^3 \quad \text{and} \quad \text{Tr} |p^0 \nabla q^0| \leq CN$$

for some  $C > 0$ , where  $p^0 = \sum_{j=1}^N |\varphi_j^0\rangle \langle \varphi_j^0|$  and  $q^0 = 1 - p^0$ .

If the system evolves in time correlations among the particles and in the radiation field emerge and the many-body state will no longer be exactly of product type. However, the structure of the state is approximately preserved in the limit  $N \rightarrow \infty$ . The fact that  $N^{-2/3} a(k)W(N^{2/3}\alpha^t)\Omega = \alpha^t(k)W(N^{2/3}\alpha^t)\Omega$  and  $N^{-2/3} a^*(k)W(N^{2/3}\alpha^t)\Omega \approx \overline{\alpha^t(k)}W(N^{2/3}\alpha^t)\Omega$  motivates to approximate the action of  $N^{-2/3}\hat{\Phi}_\Lambda$  on  $\Psi_{N,t}$  by the classical scalar field

$$(3) \quad \Phi_\Lambda(x, t) = \int d^3k \frac{1}{\sqrt{16\pi^3\omega(k)}} \mathbf{1}_{|k| \leq \Lambda}(k) \left( e^{ikx} \alpha^t(k) + e^{-ikx} \overline{\alpha^t(k)} \right).$$

The Ehrenfest equations of the field operator and the expected antisymmetrized produced state of the fermions propose to couple the scalar field to the mean electron density  $\rho^t = \sum_{i=1}^N |\varphi_i^t|^2$ . In total, this suggests that the state of the system  $\Psi_{N,t}$  at later times is approximately given by  $\bigwedge_{j=1}^N \varphi_j^t \otimes W(N^{2/3}\alpha^t)\Omega$  with  $(\varphi_1^t, \dots, \varphi_N^t, \alpha^t)$  solving the Schrödinger-Klein-Gordon equations

$$(4) \quad \begin{cases} N^{-1/3} i \partial_t \varphi_j^t(x) = (N^{-2/3}(-\Delta) + \Phi_\Lambda(x, t)) \varphi_j^t(x), & \text{for } j = 1, \dots, N, \\ i \partial_t \alpha^t(k) = N^{-1/3} \delta_N \omega(k) \alpha^t(k) + N^{-1} (2\omega(k))^{-1/2} \mathbf{1}_{|k| \leq \Lambda}(k) \mathcal{FT}[\rho^t](k), \end{cases}$$

where  $\Phi_\Lambda$  is defined as in (3).

In order to formulate the precise statement we define the  $k$ -particle reduced density matrices of the fermions by  $\gamma_{N,t}^{(k,0)} = \text{Tr}_{k+1, \dots, N} \otimes \text{Tr}_{\mathcal{F}} |\Psi_{N,t}\rangle \langle \Psi_{N,t}|$  (where  $\text{Tr}_{k+1, \dots, N}$  denotes the partial trace over the coordinates  $x_{k+1}, \dots, x_N$  and  $\text{Tr}_{\mathcal{F}}$  the trace over the Fock space) and the one-particle reduced density matrix of the bosons via the integral kernel  $\gamma_{N,t}^{(0,1)}(k, k') = N^{-4/3} \langle \Psi_{N,t}, a^*(k') a(k) \Psi_{N,t} \rangle$ . Our main theorem is the following.

**Theorem 1** (Theorem II.3. in [10]). *Let Assumption 1 be satisfied,  $\alpha^0 \in L^2(\mathbb{R}^3, (1 + k^2)dk)$ ,  $\mathcal{N} = \int d^3k a^*(k) a(k)$  and  $\Psi_{N,0} \in L^2(\mathbb{R}^{3N}) \otimes \mathcal{F} \cap \mathcal{D}(\mathcal{N}) \cap \mathcal{D}(\mathcal{NH}_N)$  with  $\|\Psi_{N,0}\| = 1$ . Moreover, let  $\Psi_{N,t}$  be the solution to (1) with initial condition  $\Psi_{N,0}$ , and  $\varphi_1^t, \dots, \varphi_N^t, \alpha^t$  be the solution to (4) with initial condition*

$\varphi_1^0, \dots, \varphi_N^0, \alpha^0$ . We define  $p^t = \sum_{j=1}^N |\varphi_j^t\rangle \langle \varphi_j^t|$ ,  $q^t = 1 - p^t$  for any  $t \in \mathbb{R}$  and

$$\begin{aligned} a_N &= \text{Tr} \left| \gamma_{N,0}^{(1,0)} - N^{-1} p^0 \right|, \\ b_N &= N^{1/3} \text{Tr}(\gamma_{N,0}^{(2,0)} q^0 \otimes q^0), \\ c_N &= N^{-1} \left\langle W^{-1}(N^{2/3} \alpha^0) \Psi_{N,0}, \mathcal{N} W^{-1}(N^{2/3} \alpha^0) \Psi_{N,0} \right\rangle. \end{aligned}$$

Let  $a_N + b_N + c_N + N^{-1} \leq N^{1/3}$ . Then there exists a constant  $C > 0$  such that

$$\begin{aligned} \text{Tr} \left| \gamma_{N,t}^{(1,0)} - N^{-1} p^t \right| &\leq \sqrt{a_N + b_N + c_N + N^{-1}} e^{e^{C\Lambda^4(1+\|\alpha^0\|_2)(1+t^2)}}, \\ \text{Tr} \left| \gamma_{N,t}^{(0,1)} - |\alpha^t\rangle \langle \alpha^t| \right| &\leq \sqrt{N^{-1/3}(a_N + b_N + c_N) + N^{-4/3}} e^{e^{C\Lambda^4(1+\|\alpha^0\|_2)(1+t^2)}} \end{aligned}$$

for any  $t \geq 0$ . In particular, for  $\Psi_{N,0} = \bigwedge_{j=1}^N \varphi_j^0 \otimes W(N^{2/3} \alpha^0) \Omega$  we have  $a_N = b_N = c_N = 0$  and one obtains

$$\begin{aligned} \text{Tr} \left| \gamma_{N,t}^{(1,0)} - N^{-1} p^t \right| &\leq N^{-1/2} e^{e^{C\Lambda^4(1+\|\alpha^0\|_2)(1+t^2)}}, \\ \text{Tr} \left| \gamma_{N,t}^{(0,1)} - |\alpha^t\rangle \langle \alpha^t| \right| &\leq N^{-2/3} e^{e^{C\Lambda^4(1+\|\alpha^0\|_2)(1+t^2)}}. \end{aligned}$$

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## Invariance Principle for Random Lorentz Gas in the Boltzmann-Grad Limit

CHRISTOPHER LUTSKO

(joint work with B. Tóth)

Consider the random Lorentz process  $t \mapsto X^{r,\rho}(t)$  with hard-core spherical scatterers of radius  $r > 0$  and density  $\rho > 0$ . Namely

- Consider a Poisson point process of intensity  $\rho$ ,  $\mathcal{P} = \mathcal{P}(\rho)$ , and a field of Poisson distributed scatterers  $\mathcal{P} + \mathcal{B}_r^d$  where  $\mathcal{B}_r^d$  denotes a ball of radius  $r$ .
- If the origin is covered by a scatterer (i.e  $0 \in \mathcal{P} + \mathcal{B}_r^d$ ), then  $X^{r,\rho}(t) = 0$  for all  $t > 0$ . (In our setting this will occur with probability tending to 0).
- If the origin is not covered by a scatterer then  $X^{r,\rho}(0) = 0$  and
- $X^{r,\rho}$  moves in straight lines with unit speed and collides elastically on the boundary of  $(\mathcal{P} + \mathcal{B}_r^d)^c$ .

An open question of significant interest is to understand the long time behavior of  $t \mapsto X^{r,\rho}(t)$  in either of the following settings:

- *Quenched Limit:* For a typical realization of the Poisson point process averaging over the initial velocity.
- *Average-Quenched Limit:* Averaging over the initial velocity *and* the Poisson configuration.

In either of these settings, the 'holy grail' of the field would be to prove an invariance principle in the *diffusive limit*:

$$(1) \quad t \mapsto \frac{X^{r,\rho}(Tt)}{\sqrt{T}} \quad \text{as } T \rightarrow \infty$$

(that is, to show that the process in (1) converges weakly to a Wiener process) (see [7] for a detailed survey).

In the periodic setting, this limit is (relatively) well understood (see the surveys [3], [5]), because of the applicability of methods from hyperbolic dynamical systems theory. However, in the random setting less is known with mathematical rigour. Gallavotti [2] showed that the Lorentz process  $t \mapsto X^{r,\rho}(t)$  obeys a linear Boltzmann equation in the Boltzmann-Grad limit. Spohn [6] then showed that the Lorentz process, in the annealed setting (and for a wide class of scatterer configurations) converges to a Markovian flight process (i.e a process moving in straight lines with instantaneous velocity jumps separated by independent exponential flight times). Then Boldrighini, Bunimovich, and Sinai [1] proved the same convergence result in the quenched setting.

*However* these results are all restricted to finite time intervals in the *Boltzmann-Grad* limit:

$$(2) \quad \begin{array}{l} \rho \rightarrow \infty \\ r \rightarrow 0 \quad \rho r^{d-1} \rightarrow \Omega_{d-1} \end{array}$$

where  $\Omega_{d-1}$  is the volume of the  $d - 1$ -dimensional ball. In this setting and on these time scales, the memory effects of the Lorentz process do not occur (with high probability).

In a recent work [4] Tóth and the author proved that, in dimension 3, in the *joint* Boltzmann-Grad and diffusive limits, the Lorentz process stays close in this particular coupling to a Markovian flight processes in the annealed sense. More precisely, given velocities, uniformly distributed on  $S^2$  (the unit sphere),  $\{v_i\}_{i=1}^\infty$  and exponentially distributed flight times  $\{\xi_i\}_{i=1}^\infty$ , denote

$$(3) \quad Y_0 = 0 \quad , \quad Y_n = \sum_{i=1}^n \xi_i v_i$$

and let  $t \mapsto Y(t)$  be the process moving with unit speed between  $Y_{i-1}$  and  $Y_i$  with velocity  $v_i$  - the Markovian flight process. In this case, with  $\rho = \Omega_{d-1} r^{-(d-1)}$  (i.e Boltzmann-Grad scaling):

**Theorem 2.** *Let  $T = T(r)$  be such that  $\lim_{r \rightarrow 0} T(r) = \infty$  and  $\lim_{r \rightarrow 0} r^2 |\log r|^2 T(r) = 0$ . Then, for any  $\delta > 0$ ,*

$$(4) \quad \lim_{r \rightarrow 0} \mathbf{P} \left( \sup_{0 \leq t \leq T} |X^{r,\rho}(t) - Y(t)| > \delta \sqrt{T} \right) = 0,$$

and hence

$$(5) \quad \left\{ t \mapsto T^{-1/2} X^{r,\rho}(Tt) \right\} \Rightarrow \{t \mapsto W(t)\},$$

as  $r \rightarrow 0$ , in the averaged-quenched sense. On the right hand side of (5)  $W$  is a standard Wiener process of variance 1 in  $\mathbb{R}^3$ .

The proof is based on probabilistic coupling. As this coupling argument is central to the proof we summarize it here. We will realize the Lorentz process as an exploration process. That is, as the  $X^{r,\rho}$  process evolves it discovers more of the environment: discovering yet-unseen scatterers with rate 1 (just like the  $Y$  process). However, the  $X^{r,\rho}$  process has a long memory and scatters off of the previously discovered scatterers (*recollisions*). Similarly, as the  $X^{r,\rho}$  process evolves it traces out a path of previously explored space, hence the new scatterers cannot be placed over the old path.

The coupling is then realized as follows, let  $U(t) = \dot{Y}(t)$  and  $V^r(t) = \dot{X}^{r,\rho}(t)$

- At time 0,  $V^r(0) = U(0)$ .
- With frequency of typical order  $r$  two kinds of *mismatches* occur, during which the two velocity processes do not coincide:
  - *Recollisions* of the Lorentz process with previously placed scatterers (hence  $V^r(t)$  changes when  $U(t)$  does not).
  - Scatterings of the Markovian flight process at a time and in a direction such that the Lorentz process would block its old path if it placed the appropriate scatterer (we call these *shadowed scatterings*). During these mismatches  $V^r(t)$  remains the same while  $U(t)$  changes.

- After a mismatch a new, jointly realized, scattering event of the two processes occurs, recoupling the two velocity processes.

To prove Theorem 2 we show that such mismatches occur with typical frequency of order  $r$ . Not only that but the mismatches are direct (i.e involve only 3 consecutive path segments of the Markovian flight process). Hence we use geometric observations to show that the typical time to recouple after a mismatch is  $EXP(1)$  distributed. With that, we show that the mismatches are well separated in time. Therefore in time  $T$  the separation is given by

$$(6) \quad \frac{|X^{r,\rho}(T) - Y(T)|}{\sqrt{T}} \leq T^{-1/2} \int_0^T |U(t) - V^r(t)| dt \\ \leq T^{-1/2}(T \cdot r) \rightarrow 0,$$

which follows since there are  $\mathcal{O}(T)$  collisions in time  $T$ , each with a probability  $r$  of being a mismatch, and the separation during each mismatch is of order  $\mathcal{O}(1)$ . Note that the log correction is not shown by this handwaving argument.

Finally (5) follows from (4) and a classical invariance principle for the process  $t \mapsto Y(t)$ .

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### On the particle approximation to stationary solutions of the Boltzmann equation

MARIO PULVIRENTI

As it is well known, the Boltzmann equation is a useful tool to understand the behaviour of a rarefied gas. From a mathematical side the study of the Boltzmann equation is mostly devoted to the initial value problem. On the other hand in most of the physical applications the solutions of the Boltzmann equation are seen in a stationary non-equilibrium regime. Indeed after a short time dependent transient,

the system has the tendency to stabilize in a non trivial stationary state which should describe transport phenomena.

The problem of the derivation of the Boltzmann equation in such a situation is much beyond our knowledge at moment. In fact even having a long time validity result (and this is not the case) we do not expect that the limits  $t \rightarrow \infty$  and  $N \rightarrow \infty$  according to the Boltzmann-Grad limit are commutable. Here  $t$  is the time and  $N$  the particle number.

Some years ago in [3] a stochastic particle system in a container with diffusive boundary with varying temperature was proven to approximate the stationary solution of the corresponding Boltzmann equation (actually the Povzner equation which is a regularization of the true Boltzmann equation). The proof works only under severe assumptions on the Maxwellian at the boundary, namely it was assumed an unphysical cutoff on small and large velocities. We discuss the possibility of removing such a cutoff in the special situation of a gas contained between two planes with diffusive boundary conditions at different temperature, assuming also the existence of a non vanishing horizontal constant external field  $\mathbf{F}$  and the intensity of the collisions among the particles sufficiently small, namely the Benard problem for a very rarefied gas [7].

More precisely we consider, as in [3], a gas modelled by a stochastic particle system which is the non-homogeneous extension of the well known Kac's model ( see [5] and [6]). The particle models we are considering is the basis for the so called direct Montecarlo simulation method [1] and [2], which is widely used for the numerical simulations of a real gas. Therefore this result can be seen as a justification of the use of such algorithm assuming "true" the Boltzmann equation which however should be still derived from mechanical particle systems.

The approximation result I am discussing can be obtained via a sequence of steps.

1) There exists a unique stationary solution of our model of Boltzmann equation  $g(x, v)$  being  $x, v$  position and velocity respectively.

2) The  $N$ -particle system has a unique invariant measure denoted by  $\tilde{f}^N$  and marginals  $\tilde{f}_k^N$ ,  $k = 1 \dots N$ .

3) The convergence result can be formulated as:  
suppose the mean-free path sufficiently large. Then for any integer  $k$ :

$$(1) \quad \|\tilde{f}_k^N - g_k\|_{L^1} \leq \frac{c_2^k}{N}$$

where  $g_k = g^{\otimes k}$ , being  $g$  the solution of the stationary Boltzmann equation and  $c_2$  some positive computable constant.

The proof is based on a careful analysis of the Knudsen flow (free particles with diffusive boundary conditions) and a precise control of the correlation error.

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**Fluctuation theory at low density**

SERGIO SIMONELLA

(joint work with T. Bodineau, I. Gallagher, L. Saint-Raymond)

The aim of this talk is to report on recent and ongoing progress on the mathematical treatment of the fluctuation theory at the kinetic scale. The focus is on analysing quantitatively the decay of correlations in the limit of low density for the hard sphere gas.

As reference model we take a three-dimensional, macroscopic box filled with hard balls of diameter  $\varepsilon \rightarrow 0$  and average number of particles increasing as  $\varepsilon^{-2}$ , so that the mean free path remains of order one. At time zero the center of the hard spheres is approximately Poisson-distributed, with density  $f_0$  arbitrarily prescribed. In particular, weak correlations are due to the condition of non-overlap among different spheres.

At leading order the dynamics is driven by the Boltzmann equation. The classical result in the field (Lanford’s theorem) is a rigorous derivation of such equation as a law large numbers for times shorter than (and order of) the mean free time. Specifically, the empirical measure on the one-particle phase space converges to the smooth Boltzmann density  $f(t)$ , with  $f(t = 0) = f_0$ , at least if the initial measure satisfies suitable uniform bounds.

Besides the purely deterministic evolution, by looking at finer scales one discovers random fluctuations, which retain a larger amount of microscopic information. This feature is understood at best by studying data far from equilibrium. At order  $\varepsilon$ , corrections are described in the physical literature by means of a stochastic PDE (“fluctuating Boltzmann”) given by a linearized (around  $f(t)$ ) Boltzmann operator, plus a Gaussian white noise in spacetime. The latter is due to characteristic dynamical events called *recollisions*, as pointed out by Herbert Spohn in 1981 in his explicit derivation of the covariance. Such collisions keep memory of the past

trajectory from time  $t$  to time zero, and their effect is visible in the nonequilibrium state.

In our contribution [3] we prove the central limit theorem for the fluctuation field of the hard sphere gas, and that the process converges to a generalized Ornstein-Uhlenbeck given by the predicted fluctuating equation. This is worked out under the same assumptions of Lanford's result (and if a central limit theorem holds at time zero). Moreover, in doing so, we optimally quantify the correlations at arbitrary order. Technically, this means that we obtain the limiting equations for the whole hierarchy of *cumulants*. These functions measure events where  $j$  particles are completely connected by chains of collisions preventing their statistical independence. As  $j$  is arbitrary, ultimately we hope to derive the probability of not only small, but also large deviations from the average profile  $f(t)$ .

The core of the work is a combinatorial problem on clusters of particles ("collision trees") connected by collision relations. The convenient quantities are the analogue of the *truncated correlation functions* commonly used in equilibrium statistical mechanics. In this connection, we stress that we consider systems in which only the average number of particles is fixed (i.e. of grand canonical type), so that the cumulants do not have a spurious part due to a given total cardinality. The cluster expansion method fits then very well with the collisional trees at low density, if combined with geometrical estimates on hard sphere trajectories.

A similar approach has been used recently (although with slightly different types of truncation) to obtain results beyond the classical one by Lanford. In [4] the truncated functions are estimated pointwise in space and up to  $j$  of polynomial order. In [1] a cumulant type expansion is crucially used to reach arbitrary times in a hard disk gas at equilibrium. Finally in [2] the cluster expansion is applied to construct counterexamples to the validity theorem and clarify the mathematical meaning of molecular chaos.

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### The Lorentz model with different scatterer distributions

BERNT WENNBERG

In this talk the Lorentz model consists of a random set of discrete points  $\Xi \subset \mathbb{R}^2$ , and a set of circular obstacles with diameter  $\varepsilon$  and center at the points,  $\bigcup_{\xi \in \Xi} B_\varepsilon(\xi)$ . Then one studies the motion  $(x(t), \phi(t))$  of a point particle where  $x(t)$  is in  $\Omega_\varepsilon$ , the whole plane except the areas covered by obstacles,  $\Omega_\varepsilon = \mathbb{R}^2 \setminus \bigcup_{x \in \Xi} B_\varepsilon(x)$ , and  $\phi(t)$

the direction of its motion. The point particle is moving with constant velocity in, and specularly reflected when hitting an obstacle.

Assuming the speed of the particle to be one, its phase space is  $\Omega_\varepsilon \times S^1$ . Let the initial position in phase space,  $(x(0), \phi(0))$  be random with density  $f_0(x, \phi)$ . Then the distribution of  $(x(t), \phi(t))$  is given by a density depending on  $\Xi$ ,  $f_\Xi(x, \phi, t)$ . Gallavotti ([5]) and later Spohn [11] proved that if  $\Xi = \Xi_\varepsilon$  is a Poisson process with intensity  $\varepsilon^{-1}$ , then  $\mathbb{E}[f_{\Xi_\varepsilon}](x, \phi, t)$  converges weakly to a density  $f(x, \phi, t)$  in  $\mathbb{R}^2$ , and that  $f$  satisfies a linear Boltzmann equation

$$(1) \quad \partial_t f(x, \phi, t) + \omega \cdot \nabla_x f(x, \phi, t) = \int_{S^1} f(x, \phi', t) |\phi \cdot \omega| d\omega - f(x, \phi, t),$$

where  $\phi'$  is the angle resulting from a specular reflection. This is the equation for a random flight process, where  $(x(t), \phi(t))$  moves an exponentially distributed distance (or time) along a straight line, and then the velocity jumps to a new random direction,  $\phi' \mapsto \phi$ , independently of the free flight time.

Contrary to this, it is possible to prove that when  $\Xi_\varepsilon$  is a regular lattice with parameter  $\varepsilon^{1/2}$ , which gives the same average number of obstacles per unit area as a Poisson process with intensity  $\varepsilon^{-1}$ , the corresponding family of functions  $f_{\Xi_\varepsilon}$  do not converge to a solution of (1). In fact the free flight times  $T$  of the limiting dynamics are not exponentially distributed, but decay as  $t^{-1}$  (i.e.,  $\mathbb{P}[T > t] \sim 1/t$ ) (see [1, 6]). However, by a suitable extension the phase space, it is possible to derive a kinetic equation (see e.g. [3, 8]).

With these two examples in mind, it is natural to investigate what properties family of point processes  $\Xi_\varepsilon$  must satisfy to obtain (1) in the limit when  $\varepsilon \rightarrow 0$ . Gallavotti's proof is carried out by a change of variables which identifies the sequence of free paths and velocity jumps of the process generated by (1) and a Poisson point process, and hence that in some  $\Xi_\varepsilon$  must asymptotically be a Poisson process with the right density; it is not so clear in which sense that should be interpreted, however, and I have seen no mathematical statement of this.

But one may study other examples of point processes. One such example is a diluted regular lattice: Let  $\Xi_\varepsilon$  be a regular lattice with parameter  $\varepsilon^{\frac{1+\delta}{2}}$ . This gives a lattice that is too dense to yield (1), the free flight times would converge to zero when  $\varepsilon \rightarrow 0$ . But the density  $\varepsilon^{-1}$  can be recovered by removing obstacles independently with probability  $1 - \varepsilon$ . Caglioti et. al. [2] proved that this model results in the linear Boltzmann equation (1) in the case  $\delta = 1$ , and the same result is actually true for any  $\delta > 0$  (see ([10])). Perhaps this result is not surprising, these  $\Xi_\varepsilon$  are asymptotically Poisson distributions in a rather strong sense, but the proof is anyway carried out by explicit calculations.

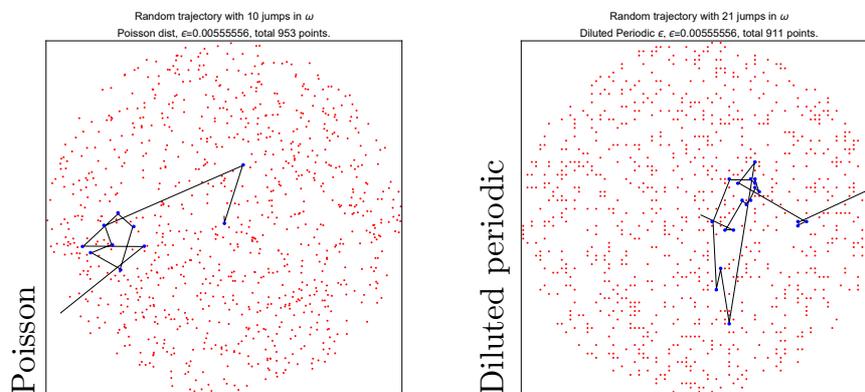
Quasi crystals give examples of non-periodic point distributions that fail to yield (1), and because the mean free paths decay as  $t^{-1}$ , just as in the periodic case. A first numerical study of this can be found in ([12]), and then a rigorous study was carried out in ([9]). Both the periodic setting and the quasi crystals are point distributions with very long range correlations.

It is most natural to consider point processes that at least in the limit are invariant under translations and rotations, and asymptotically the intensity should be

$\varepsilon^{-1}$ . The examples given above all satisfy these properties, but there are other examples: Cox processes which are Poisson point processes where the intensity itself is random, given by a Gaussian random field, for example (see [4]). Determinantal and permanental processes with kernel  $K$  are simple point processes whose intensity functions for  $n$  points  $x_1, \dots, x_n$  are given by  $\rho_n(x_1, \dots, x_n) = \det(K(x_i, x_j))$  or  $\rho_n(x_1, \dots, x_n) = \text{per}(K(x_i, x_j))$ , respectively. The determinantal processes avoid clustering of points, whereas the points in a permanental process are more clustered than the Poisson process.

Another interesting example is the set of zeros of Gaussian Analytic Functions (GAF), which are described in [7] (there are also examples of determinantal and permanental point processes in this reference). Essentially only one particular case of such functions are relevant here: Let  $(\xi_k)_{k=0}^{\infty}$  be a sequence of i.i.d. standard complex Gaussian R.V., and set  $f(z) = \sum_{k=0}^{\infty} \frac{\xi_k}{\sqrt{k!}} z^k$ . The resulting point process is like the determinantal process in that it avoids clustering of the points.

Here I present some numerical illustrations of the above models for the Poisson process, for a diluted lattice, for a point set given by a Penrose tiling, and finally, for the zero set of a GAF. For the four different cases I have generated approximately  $10^3$  points in a disk of radius 30 (in Fig. 1), or 100000 points in a disk of radius 300 (Fig. 2), and analysed trajectories of point starting with random direction from a random point close to the origin. Figure. 1 illustrates the difference between the obstacle distributions, and just one random trajectory for each case. And Figure 2 shows the distribution of free path lengths, again computed from a large number of trajectories with random initial points. Three of the four examples are very similar, but the Penrose tiling differs, according to the rigorous results that have been obtained for the Poisson distribution, the diluted periodic and for quasi crystals. There is no result for the GAF zero distribution, but judging from this simulation, it is very similar to the Poisson distribution: even if locally the point distribution avoids clustering of points, the correlation decays rapidly, and therefore in the present limit the behaviour is like the Poisson process. A more careful analysis of this is work in progress.



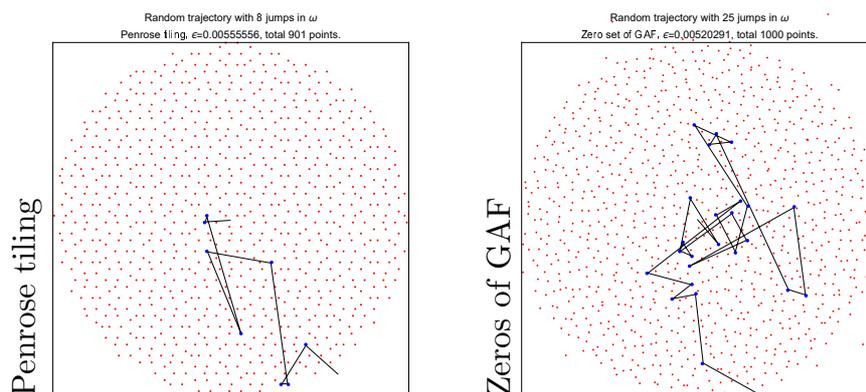


FIGURE 1. Obstacle configurations with a typical trajectory ( $10^3$  obstacles in a disk of radius 30,  $\varepsilon = 5 \times 10^{-3}$ )

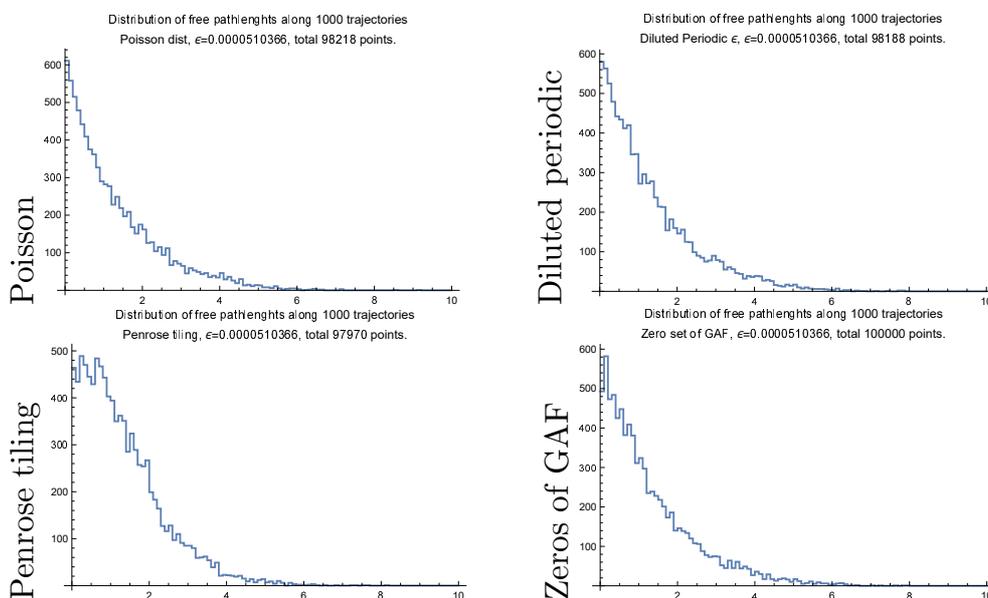


FIGURE 2. Free path lengths computed from 1000 trajectories, ( $10^5$  obstacles in a disk of radius 300,  $\varepsilon = 5 \times 10^{-5}$ )

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## Kinetic description of a Rayleigh Gas with annihilation

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(joint work with B. Lods, A. Nota)

We consider the dynamics of a tagged point particle in a gas of moving hard-spheres that are non-interacting among each other. This model is known as the ideal Rayleigh gas.

The tagged particle is initially placed at a random position  $(x_0, v_0) \in \mathbb{R}^3 \times \mathbb{R}^3$  according to some probability density  $f_0(x, v)$ .

The background gas is given by a grand-canonical ensemble  $(c_j, w_j)_{j \in J} \subset \mathbb{R}^3 \times \mathbb{R}^3$  in the phase space, where the velocity  $w_j$  of the obstacles  $(c_j, w_j)$  is distributed according to Maxwellian distribution  $\mathcal{M}_\beta(v)$  with inverse temperature  $\beta > 0$ . The radius  $\epsilon > 0$  of the obstacles will be used as a scaling parameter. The density  $\mu_\epsilon$  of particles is given by the Boltzmann-Grad scaling, i.e.:

$$\mu_\epsilon = \epsilon^{-2} \mu, \quad \text{for some } \mu > 0.$$

To this model we add the possibility of annihilation, to be able to describe systems without mass conservation, e.g. due to chemical reactions. To this end, each obstacle is assigned a Boolean variable  $z_j \in \{0, 1\}$  which determines whether it is annihilating ( $z_j = 0$ ) with probability  $\alpha \in [0, 1]$ , or elastic ( $z_j = 1$ ) with probability  $1 - \alpha$ .

Given the initial values  $(x_0, v_0)$  and  $(c_j, w_j, z_j)_{j \in J}$ , the dynamics of the system is given by the collisions between the tracer particle and an obstacle. If the particle is elastic, the velocities are updated by the hard-sphere collision rule:

$$\begin{aligned} v(t) &= v(t_-) - \frac{1}{\epsilon^2} (v(t_-) - w_j(t_-)) \cdot (x(t_-) - c_j(t_-)) (x(t_-) - c_j(t_-)), \\ w_j(t) &= v(t_-) - \frac{1}{\epsilon^2} (v(t_-) - w_j(t_-)) \cdot (x(t_-) - c_j(t_-)) (x(t_-) - c_j(t_-)), \end{aligned}$$

If the obstacle is annihilating, the tracer particle is removed from the system. In this way obtain an evolution for the probability density  $f(t, x, v)$  of the tracer

particle. We prove rigorously the convergence of  $f_\epsilon$  to a solution  $f$  of the Rayleigh-Boltzmann equation:

$$(1) \quad \partial_t f + v \cdot \nabla_x f + \mu\alpha\lambda(v)f = \mu(1 - \alpha)Q(\mathcal{M}_\beta, f).$$

Here the collision operator  $Q(\mathcal{M}_\beta, f)$  and the collision frequency  $\lambda(v)$  are given by:

$$Q(\mathcal{M}_\beta, f)(v) = \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} [(v - v_1) \cdot \hat{n}]_+ (\mathcal{M}_\beta(v'_1)f(v') - \mathcal{M}_\beta(v_1)f(v)) dv_1 d\hat{n},$$

$$\lambda(v) = \lambda_0 \int_{\mathbb{R}^3} dv_1 \mathcal{M}_\beta(v_1) |v - v_1|, \quad \lambda_0 = \int_{\mathbb{S}^2} d\hat{n} [\hat{n} \cdot \hat{v}]_+, \quad \hat{v} \in \mathbb{S}^2,$$

Moreover, we give explicit algebraic error bounds, that allow to consider hydrodynamic limits of the model.

Without quantitative bounds, the convergence has been shown in [1] and [4]. For the nonideal Rayleigh gas, that is for a tracer particle in an interacting heat bath, the convergence has been shown in [2].

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